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Proton assignments for the oxidized yeast iso-ferricytochrome *c* at 303 K
Note: The underlined chemical shift values indicate the stereospecific assignments for disastereotopic pairs of methylene protons or isopropyl methyl groups.

residue	HN	α	β	others
THR--5				
GLU--4				
PHE--3	8.68	4.34	2.59, 2.92	δ 6.95; ε 7.20, ζ 7.09
LYS--2	6.63	3.84	1.27, 1.35	γ 1.16; δ 1.48, 1.52; ε 2.85
ALA--1	7.68	3.64	1.27	
GLY-1	8.06	3.43, 4.32		
SER-2	9.40	4.73	3.41, 3.63	
ALA-3	9.03	3.97	1.50	
LYS-4	8.10			
LYS-5	7.67	4.03	1.70	γ 0.86
GLY-6	8.70	3.28, 4.02		
ALA-7	8.00	2.39	1.22	
THR-8	7.21	3.90	4.19	γCH_3 1.22
LEU-9	7.83	3.82	1.81	γ 1.49; δCH_3 0.57, 0.79
PHE-10	8.67	3.54	2.78, 3.02	δ 7.20; ε 7.79, ζ 8.47
LYS-11	8.46	4.37	1.82, 2.18	γ 1.48
THR-12	7.92	4.37	4.21	γCH_3 1.31
ARG-13	8.25	4.58	1.00,1.38	γ 1.24, 1.65
CYS-14	7.90	1.45	2.66, 2.94	
LEU-15	8.14	6.20	2.18, 2.57	γ 2.37; δCH_3 1.46; 2.04
GLN-16	9.99	4.73	2.44, 2.73	γ 2.85, 3.00;ε 6.86, 7.56
CYS-17	9.71	6.13	2.23, 2.46	
HIS-18	11.18	8.82	8.77, 14.78	δNH 12.3; δ 24.0; ε -25.1
THR-19	10.23	6.17	5.41	γCH_3 2.14
VAL-20	9.00	4.91	2.16	γCH_3 0.94
GLU-21	9.58	4.52	2.18, 2.23	
LYS-22	9.06	3.71		
GLY-23	9.53	3.72, 4.08		
GLY-24	8.32	3.71, 4.41		
PRO-25		4.54	2.18, 2.34	γ 2.56; δ 3.64
HIS-26		5.07	2.80, 3.12	δCH 6.99; εCH 7.69
LYS-27	8.32	4.71	1.81, 2.48	
VAL-28	7.52	3.08	1.30	γCH_3 -0.38, 0.82
GLY-29	7.67	-0.27, -2.89		
PRO-30		3.86	-0.20, 1.34	γ -0.23, -0.66; δ -1.36, -5.11
ASN-31	11.68	5.86	2.60, 2.93	δNH 8.16, 8.68
LEU-32	9.59	4.74	1.99, 2.39	δCH_3 0.90, 1.43
HIS-33	8.16	4.17	3.17, 3.28	
GLY-34	9.06	3.67, 3.77		
ILE-35	7.03	3.66	1.56	γ 0.48, 1.08; γCH_3 0.00; δCH_3 0.12
PHE-36	7.74	4.12	2.85, 2.89	δ 6.97; ε 6.44; ζ 6.45
GLY-37	8.76	3.64, 4.22		

ARG-38	7.88	4.65	1.82	γ 1.97; δ 3.24
HIS-39	8.07	5.17	2.71, 2.90	δCH 6.66; εCH 7.84
SER-40	8.71	4.52	3.62, 4.15	
GLY-41	8.91	1.07, 3.08		
GLN-42	7.80	4.46	1.69, 2.41	γ 2.11, 2.22; ε 6.73, 7.26
ALA-43	8.07	4.33	1.42	
GLU-44	8.79	4.12	2.09, 2.40	γ 2.33
GLY-45		3.72, 4.29		
TYR-46	6.94	3.69	0.62, 1.61	δ 4.65, 5.74; ε 3.67, 5.06
SER-47		4.10	2.99, 3.18	
TYR-48	7.75	4.18	2.44, 3.23	δ 6.97
THR-49	9.63	4.18	4.62	γCH_3 1.47
ASP-50	8.61	4.36	2.57, 2.64	
ALA-51	7.80	4.13	1.63	
ASN-52	8.34	4.63	2.90, 3.17	δNH 7.08, 7.37
ILE-53	7.63	3.65	1.87	γ 1.05, 1.57; γCH_3 0.87; δCH_3 0.87
LYS-54	9.03	4.14	1.60, 1.86	
LYS-55	7.38	4.06	1.97, 2.06	γ 1.38
ASN-56	7.34	4.37	2.30, 3.01	δNH 6.47, 7.52
VAL-57	7.33	4.15	1.36	γCH_3 0.17, 0.38
LEU-58	8.20	3.82	0.86, 1.50	γ 0.97; δCH_3 0.60, 0.32
TRP-59	7.88	4.91	2.39, 3.57	δ 6.88; ε 7.51; εNH 8.86; ζ 6.69, 7.53; η 6.48
ASP-60	9.98	4.79		
GLU-61	9.99	3.38	1.14, 1.33	γ 0.87
ASN-62	8.19	4.54	2.87, 2.92	δNH 7.11, 7.74
ASN-63	9.44	4.57	2.89, 3.25	δNH 7.00, 7.30
MET-64	8.75	4.34	2.19, 2.38	γ 1.74
SER-65	7.46	3.54	3.84, 4.16	
GLU-66	7.66	3.88	1.98, 2.11	γ 2.25, 2.44
TYR-67	8.42	4.20	3.05, 3.31	δ 7.51; ε 7.77
LEU-68	8.17	2.95	0.11, 1.09	γ 0.74, δCH_3 -0.84, -3.04
THR-69	7.44	3.85	4.33	γCH_3 1.17
ASN-70	6.83	4.97	3.14, 3.29	δNH 7.08, 8.02
PRO-71		5.69	5.03, 5.65	γ 2.26, 4.54; δ 2.83, 3.90
TML-72	9.41	5.21	2.62	γ 1.37, 2.38; ε 3.98; $-(CH_3)_3$ 3.31
LYS-73	7.89	4.55	2.06, 2.16	γ 1.71; δ 1.93; ε 3.21
TYR-74	8.23	4.76	3.93, 4.18	δ 7.87; ε 6.98
ILE-75	9.52	4.79	3.44	γ 1.55, 3.10; γCH_3 1.30; δCH_3 2.02
PRO-76		5.18	2.10, 2.61	γ 2.31; δ 3.81
GLY-77	9.33	3.99; 4.61		
THR-78	9.03	5.17	5.78	γCH_3 3.36, OH 9.71
LYS-79	8.05	4.83	1.38, 1.72	γ 0.16, 1.03; δ 0.70; ε 2.09, 2.33
MET-80	8.86			γ -30.2; ε -22.4
ALA-81	8.07	5.14	1.28	
PHE-82	8.71	4.86	2.76, 3.09	ζ 5.87; QR 6.20
GLY-83				
GLY-84		3.09, 4.46		
LEU-85	8.10	4.34	0.84, 1.09	γ 0.91; δCH_3 0.03, 0.40

LYS-86	8.37	3.91	1.62, 1.81	γ 1.42
LYS-87	8.72	4.35	1.47, 1.68	
GLU-88	8.86	3.40	1.86, 2.06	
LYS-89	8.58	3.85	1.59, 1.73	
ASP-90	6.25	4.06	2.21, 2.64	
ARG-91	7.25	3.26	1.86	
ASN-92	8.51	3.84	2.62, 2.82	δNH 6.97, 7.18
ASP-93	8.52	4.06	2.45, 2.65	
LEU-94	8.16	3.82	1.30, 1.36	γ 0.96; δCH_3 0.04, 0.40
ILE-95	8.70	3.05	1.76	γ 0.32, 1.39; γCH_3 0.24; δCH_3 0.55
THR-96	7.96	3.72	4.27	γ 1.15
TYR-97	7.69	4.06	2.90, 3.52	δ 5.74, 6.72; ε 7.16, 7.64
LEU-98	8.97	3.26	1.31, 1.80	γ 1.43; δCH_3 0.12, 0.31
LYS-99	8.63	3.47	1.18, 1.49	γ 0.65; δ 0.80
LYS-100	6.63	4.14	1.43, 1.79	
ALA-101	8.39	4.04	0.71	
SER-102	7.67		3.24	
GLU-103	6.93	4.10	2.02, 2.32	

Heme Assignments

QM5 10.98 QM8 34.70 QM1 8.01 QM3 31.03 HDM 2.34 QT2 -2.10 HT2A -0.70 HAM 2.66 QT4 2.08 HT4A 2.86 HBM 1.71 HP61 2.88, HP62 -1.43, HP63 1.03 HP64 2.66 HGM 8.03 HP71 12.72, HP72 15.91, HP73 1.34 HP74 -0.23

Experimental NOE intensities used for the structural calculation. Note: an asterisk mark (*) indicates the intensities of the peaks that correspond to two or more protons with degenerate chemical shifts are divided by the number of protons they contain.

-3 PHE						HZ	-1 ALA	QB	38176.0
						HZ	95 ILE	HB	13152.0
	HN	-3 PHE	HB2	11496.0		HZ	95 ILE	QG2	25736.0
	HN	-3 PHE	HB3	38340.0		HZ	96 THR	HA	32760.0
	HA	-3 PHE	CG	41680.0*2		HZ	96 THR	QG2	12776.0
	HA	-2 LYS+	HN	10455.0	-2 LYS+				
	HB2	-3 PHE	CG	56920.0*2		HN	-2 LYS+	HA	8030.0
	HB3	-3 PHE	CG	106680.0*2		HN	-2 LYS+	HB3	22045.0
	HB3	65 SER	HB2	23192.0		HN	-2 LYS+	HG2	11745.0
	CG	-3 PHE	CZ	25020.0*2*2		HN	-1 ALA	HN	3033.6
	CG	61 GLU-	HB2	10684.0*2		HA	-2 LYS+	HB2	54592.0
	CG	61 GLU-	HB3	13592.0*2		HA	-2 LYS+	HG2	39696.0
	CG	61 GLU-	HG2	4303.2*2		HA	-2 LYS+	HD2	39672.0
	CG	65 SER	HB2	4168.0*2		HA	-1 ALA	HN	16944.0
	CG	95 ILE	HB	11560.0*2		HB2	92 ASN	HD21	25555.0
	CG	95 ILE	QG2	9072.0*2		HB3	92 ASN	HD21	32045.0
	CG	95 ILE	QD1	11968.0*2	-1 ALA				
	CZ	-3 PHE	HZ	29556.0*2		HN	-1 ALA	HA	4915.0
	CZ	-1 ALA	HA	14952.0*2		HN	-1 ALA	QB	142050.0
	CZ	-1 ALA	QB	24776.0*2		HA	-1 ALA	QB	213520.0
	CZ	92 ASN	HB3	11168.0*2		HA	1 GLY	HN	23245.0
	CZ	95 ILE	HB	43720.0*2		QB	1 GLY	HN	38030.0
	CZ	95 ILE	QG2	18608.0*2	1 GLY				
	CZ	95 ILE	QD1	1012.2*2		HN	1 GLY	HA1	36995.0
	CZ	96 THR	HN	8040.0*2		HN	96 THR	QG2	14120.0
	CZ	99 LYS+	HD3	5548.0*2		HA1	92 ASN	HB2	52016.0
	HZ	-1 ALA	HA	74712.0		HA2	2 SER	HN	12996.0

	HA2	96	THR	QG2	156880.0
2 SER					
	HN	2	SER	HA	110940.0
	HN	2	SER	HB2	12996.0
	HN	2	SER	HB3	8911.2
	HN	3	ALA	HN	5799.6
	HN	93	ASP-	HA	5691.6
	HN	93	ASP-	HB2	4160.4
	HA	3	ALA	HN	504960.0
	HA	4	LYS+	HN	6845.0
	HB3	3	ALA	HN	17424.0
3 ALA					
	HN	3	ALA	HA	27204.0
	HN	3	ALA	QB	54200.0
	HN	4	LYS+	HN	6980.0
	HA	3	ALA	QB	319840.0
	HA	6	GLY	HA2	64456.0
	HA	96	THR	HB	7572.0
	HA	96	THR	QG2	28304.0
	HA	97	TYR	HB3	14352.0
	QB	4	LYS+	HN	73728.0
4 LYS+					
	HN	5	LYS+	HN	5645.0
5 LYS+					
	HN	5	LYS+	HA	75384.0
	HN	5	LYS+	HB2	64900.0
	HN	5	LYS+	HG2	5724.0
	HA	6	GLY	HN	17232.0
	HA	8	THR	QG2	36384.0
	HB3	6	GLY	HN	121680.0
	HB3	93	ASP-	HB3	51984.0
	HG2	93	ASP-	HB3	53316.0
6 GLY					
	HN	6	GLY	HA1	102204.0
	HN	6	GLY	HA2	59952.0
	HN	7	ALA	HN	34524.0
	HN	8	THR	HN	4701.6
	HN	93	ASP-	HB3	25224.0
	HA1	7	ALA	HN	34308.0
	HA1	9	LEU	HB3	77368.0
	HA1	9	LEU	HG	74232.0
	HA1	9	LEU	QD2	105280.0
	HA1	10	PHE	HN	17664.0
	HA1	93	ASP-	HB3	106240.0
	HA2	7	ALA	HN	2930.4
	HA2	9	LEU	HN	820.0
	HA2	9	LEU	HB3	6798.0
	HA2	9	LEU	QD2	14936.0
	HA2	93	ASP-	HB3	12036.0
	HA2	94	LEU	HA	189840.0
	HA2	94	LEU	QD1	2296.8
7 ALA					
	HN	7	ALA	HA	45140.0
	HN	7	ALA	QB	197650.0
	HN	8	THR	HN	41950.0
	HN	97	TYR	HB2	6709.2
	HN	97	TYR	HB3	3222.0
	HA	7	ALA	QB	218960.0
	HA	8	THR	HN	7740.0
	HA	10	PHE	HN	18564.0
	HA	10	PHE	HB2	19728.0
	HA	10	PHE	HB3	24904.0
	QB	8	THR	HN	35185.0
	QB	8	THR	HA	6748.0
8 THR					
	HN	8	THR	HA	11255.0
	HN	8	THR	HB	33192.0
	HN	8	THR	QG2	183050.0
	HN	9	LEU	HN	35688.0
	HN	10	PHE	HN	12060.0
	HA	8	THR	HB	159760.0
	HA	8	THR	QG2	94720.0
	HA	9	LEU	HN	3315.0
	HA	10	PHE	HN	2370.0
	HA	11	LYS+	HN	20110.0
	HA	11	LYS+	HB2	195760.0
	HA	11	LYS+	HB3	30744.0
	HA	11	LYS+	QG	34756.0*2
	HA	11	LYS+	QD	3657.2*2
	HB	8	THR	QG2	162080.0
	HB	9	LEU	HN	18912.0
	HB	11	LYS+	HG2	7306.8
	HB	12	THR	QG2	26808.0
	QG2	9	LEU	HN	8779.2
	QG2	11	LYS+	HN	3682.8
9 LEU					
	HN	9	LEU	HA	22356.0
	HN	9	LEU	HB3	65600.0
	HN	9	LEU	HG	20064.0
	HN	9	LEU	QD1	14270.0
	HN	9	LEU	QD2	53350.0
	HN	10	PHE	HN	44688.0
	HN	11	LYS+	HN	18336.0
	HA	9	LEU	HB3	17376.0
	HA	9	LEU	HG	26560.0
	HA	9	LEU	QD1	121360.0
	HA	9	LEU	QD2	79816.0
	HA	10	PHE	HN	15120.0
	HA	12	THR	HN	16955.0
	HA	13	ARG+	HB2	7360.8
	HB3	9	LEU	HG	98320.0
	HB3	9	LEU	QD1	38696.0
	HB3	9	LEU	QD2	213840.0
	HB3	10	PHE	HN	46705.0
	HB3	94	LEU	QD2	3680.4
	HG	9	LEU	QD1	133440.0
	HG	9	LEU	QD2	252560.0
	HG	10	PHE	HN	2830.8
	HG	94	LEU	QD2	16284.0
	QD1	13	ARG+	HG2	12636.0
	QD1	13	ARG+	HG3	16368.0
	QD1	85	LEU	QD1	47496.0
	QD1	90	ASP-	HB2	47248.0
	QD1	94	LEU	QD1	44016.0
	QD1	94	LEU	QD2	37968.0
	QD2	10	PHE	HN	35495.0
	QD2	85	LEU	QD1	26904.0
	QD2	85	LEU	QD2	21336.0
	QD2	90	ASP-	HA	79600.0
	QD2	90	ASP-	HB2	116320.0
	QD2	90	ASP-	HB3	9444.0
	QD2	93	ASP-	HB3	25548.0
	QD2	94	LEU	HN	20316.0
	QD2	94	LEU	HB2	73320.0
	QD2	94	LEU	QD1	6103.2
10 PHE					
	HN	10	PHE	HA	44736.0
	HN	10	PHE	HB2	38220.0
	HN	10	PHE	HB3	62076.0
	HN	11	LYS+	HN	44808.0
	HN	12	THR	HN	13930.0
	HN	13	ARG+	HN	7865.0
	HN	94	LEU	QD2	28075.0
	HA	10	PHE	HB2	49144.0
	HA	10	PHE	HB3	6219.2
	HA	10	PHE	CG	16428.0*2
	HA	11	LYS+	HN	3560.0
	HA	13	ARG+	HN	3600.0
	HA	13	ARG+	HB2	37216.0
	HA	14	CYSS	HN	12048.0
	HA	15	LEU	HN	9780.0
	HA	94	LEU	QD1	43912.0
	HA	94	LEU	QD2	23376.0
	HB2	10	PHE	CG	13144.0*2
	HB2	11	LYS+	HN	14520.0
	HB2	94	LEU	QD2	18256.0
	HB2	97	TYR	HE1	20600.0
	HB2	98	LEU	QD2	18752.0
	HB3	10	PHE	CG	51680.0*2
	HB3	10	PHE	HD2	23960.0
	HB3	11	LYS+	HN	53976.0
	HB3	11	LYS+	QG	34700.0*2
	HB3	94	LEU	QD2	2775.2
	HB3	97	TYR	HE1	17136.0
	CG	10	PHE	CZ	45580.0*2*2
	CG	10	PHE	HZ	14536.0*2
	CG	11	LYS+	HN	13530.0*2
	CG	11	LYS+	HA	38792.0*2
	CG	14	CYSS	HB2	4532.0*2
	CG	15	LEU	HN	5860.0*2
	CG	15	LEU	HA	1991.6*2
	CG	15	LEU	HB2	17988.0*2
	CG	15	LEU	QD1	8240.0*2
	CG	15	LEU	QD2	20296.0*2

	CG	18	HEM	QM1	26728.0*2
	CG	94	LEU	QD2	22760.0*2
	CG	98	LEU	QD1	7768.0*2
	CG	98	LEU	QD2	31052.0*2
	CZ	10	PHE	HZ	49520.0*2
	CZ	15	LEU	HA	8256.0*2
	CZ	15	LEU	HB2	6728.0*2
	CZ	15	LEU	QD1	22940.0*2
	CZ	18	HEM	HB2	1397.2*2
	CZ	18	HEM	HB3	1901.2*2
	CZ	19	THR	HA	4752.0*2
	CZ	20	VAL	QQG	3680.0*2*2
	CZ	32	LEU	QD1	5304.0*2
	CZ	98	LEU	QD1	3287.6*2
	CZ	98	LEU	QD2	8356.0*2
	HZ	14	CYSS	HB3	3305.6
	HZ	15	LEU	HA	10968.0
	HZ	15	LEU	QD1	12640.0
	HZ	18	HEM	HA	5920.8
	HZ	18	HEM	HB2	11568.0
	HZ	18	HEM	HB3	41720.0
	HZ	19	THR	HA	38720.0
	HZ	20	VAL	HA	4096.8
	HZ	20	VAL	HB	27168.0
	HZ	20	VAL	QQG	30280.0*2
	HZ	32	LEU	QD1	37008.0
11 LYS+					
	HN	11	LYS+	HA	41952.0
	HN	11	LYS+	HB2	155760.0
	HN	11	LYS+	HB3	28068.0
	HN	11	LYS+	HG2	5559.6
	HN	12	THR	HN	48048.0
	HA	11	LYS+	HB2	62896.0
	HA	11	LYS+	HB3	26008.0
	HA	11	LYS+	HG2	47508.0
	HA	12	THR	HN	13056.0
	HA	15	LEU	HN	27192.0
	HA	15	LEU	HB2	334800.0
	HA	15	LEU	HB3	86080.0
	HA	15	LEU	QD1	21944.0
	HA	15	LEU	QD2	88400.0
	HB2	11	LYS+	HG2	20616.0
	HB2	12	THR	HN	40104.0
	HB3	11	LYS+	HG2	139200.0
	HG2	15	LEU	HB2	25548.0
	HG2	15	LEU	QD1	116796.0
12 THR					
	HN	12	THR	HA	30960.0
	HN	12	THR	HB	18480.0
	HN	12	THR	QG2	71150.0
	HN	13	ARG+	HN	88248.0
	HA	12	THR	HB	72880.0
	HA	12	THR	QG2	116240.0
	HA	13	ARG+	HN	1424.4
	HB	12	THR	QG2	145760.0
	HB	13	ARG+	HN	6073.2
13 ARG+					
	HN	13	ARG+	HA	32760.0
	HN	13	ARG+	HB2	81216.0
	HN	13	ARG+	HB3	19440.0
	HN	13	ARG+	HG2	16800.0
	HN	13	ARG+	HG3	25248.0
	HN	14	CYSS	HN	101550.0
	HA	13	ARG+	HB2	23848.0
	HA	13	ARG+	HB3	91920.0
	HA	14	CYSS	HN	9254.4
	HA	18	HEM	QT2	4077.6
	HB2	14	CYSS	HN	4630.8
	HB2	18	HEM	HT2A	17928.0
	HB2	18	HEM	QT2	29928.0
	HB2	82	PHE	HZ	12696.0
	HB2	82	PHE	QR	6489.6*5
	HB3	14	CYSS	HN	2704.8
	HB3	18	HEM	HT2A	22416.0
	HB3	18	HEM	QT2	50704.0
	HB3	82	PHE	HZ	9976.0
	HB3	82	PHE	QR	13875.2*5
14 CYSS					
	HN	14	CYSS	HA	29184.0
	HN	15	LEU	HN	123000.0
	HA	14	CYSS	HB3	174840.0
	HA	15	LEU	HN	32688.0
	HA	18	HEM	HT2A	18840.0
	HA	18	HEM	QT2	31524.0
	HB2	18	HEM	HT2A	17656.0
	HB3	15	LEU	HN	10308.0
	HB3	15	LEU	HA	19984.0
	HB3	18	HEM	QM1	6964.8
	HB3	18	HEM	QT2	4766.4
	HB3	18	HEM	HAM	8568.0
15 LEU					
	HN	15	LEU	HA	32400.0
	HN	15	LEU	HB2	77256.0
	HN	15	LEU	HB3	91800.0
	HN	15	LEU	HG	4370.0
	HN	15	LEU	QD1	8949.6
	HN	15	LEU	QD2	22630.0
	HA	15	LEU	HB2	178240.0
	HA	15	LEU	HB3	86600.0
	HA	15	LEU	HG	56992.0
	HA	15	LEU	QD1	198400.0
	HA	15	LEU	QD2	28080.0
	HA	17	CYSS	HN	13884.0
	HA	18	HEM	HN	48348.0
	HA	18	HEM	HB2	6459.2
	HB2	15	LEU	QD2	62520.0
	HB3	15	LEU	QD2	87696.0
	HG	15	LEU	QD1	226880.0
	HG	15	LEU	QD2	217280.0
	QD1	19	THR	HA	79184.0
16 GLN					
	HN	16	GLN	HB2	68688.0
	HN	16	GLN	HB3	17920.0
	HN	16	GLN	HG2	10890.0
	HN	16	GLN	HG3	92400.0
	HN	17	CYSS	HN	18585.0
	HB2	17	CYSS	HN	11025.0
	HB3	17	CYSS	HN	46510.0
	HG2	16	GLN	HE21	11175.0
	HG2	17	CYSS	HN	16980.0
	HG3	16	GLN	HE21	7660.0
17 CYSS					
	HN	17	CYSS	HA	42780.0
	HN	17	CYSS	HB2	12768.0
	HN	18	HEM	HN	206640.0
	HA	17	CYSS	HB2	70272.0
	HA	17	CYSS	HB3	69192.0
	HA	18	HEM	HN	22032.0
	HA	28	VAL	HB	135120.0
	HA	28	VAL	QG1	26872.0
	HA	28	VAL	QG2	43328.0
	HA	29	GLY	HN	13435.0
	HB2	18	HEM	QM3	6006.4
	HB2	18	HEM	HT4A	31608.0
	HB2	29	GLY	HN	11522.4
	HB3	18	HEM	HT4A	42736.0
	HB3	18	HEM	HBM	46016.0
	HB3	28	VAL	HB	21936.0
	HB3	28	VAL	QG1	5132.8
	HB3	28	VAL	QG2	45296.0
	HB3	29	GLY	HA2	3520.8
18 HEM					
	HN	18	HEM	HA	28620.0
	HN	18	HEM	HB2	21365.0
	HN	18	HEM	HB3	12336.0
	HN	19	THR	HA	4410.0
	HA	18	HEM	HB3	95520.0
	HA	19	THR	HN	183840.0
	HA	19	THR	HA	6544.0
	HA	31	ASN	HA	11424.0
	HB2	19	THR	HN	17928.0
	HB2	32	LEU	QD1	7375.2
	HB3	19	THR	HN	35015.0
	HB3	19	THR	HA	5244.8
	HB3	32	LEU	HN	4842.0
	HB3	32	LEU	HB3	2514.4
	HB3	32	LEU	HG	29128.0
	HB3	32	LEU	QD1	22224.0
	HB3	32	LEU	QD2	1553.6
	HAP71	18	HEM	HAP72	283950.0
	HAP71	18	HEM	HBP73	46040.0
	HAP71	18	HEM	HBP74	42576.0
	HAP71	18	HEM	QM8	8808.0
	HAP71	18	HEM	HGM	33248.0

HAP71	18	HEM	HAP61	1193.6
HAP71	18	HEM	HBP64	1150.4
HAP71	35	ILE	HG12	4589.6
HAP71	52	ASN	HD21	2305.0
HAP71	52	ASN	HD22	20030.0
HAP71	59	TRP	HZ2	43192.0
HAP72	18	HEM	HBP73	43576.0
HAP72	18	HEM	HBP74	36128.0
HAP72	18	HEM	QM8	20792.0
HAP72	18	HEM	HGM	12344.0
HAP72	35	ILE	HG12	10488.0
HAP72	52	ASN	HD22	17855.0
HAP72	59	TRP	HE1	26560.0
HAP72	59	TRP	HZ2	102800.0
HAP72	59	TRP	HH2	6636.0
HBP73	18	HEM	HBP74	491900.0
HBP73	18	HEM	QM8	17928.0
HBP73	30	PRO	HG2	35856.0
HBP73	35	ILE	HG12	34064.0
HBP74	18	HEM	QM8	7816.8
HBP74	18	HEM	HGM	2682.0
HBP74	30	PRO	HG2	151600.0
HBP74	30	PRO	HD3	20775.0
HBP74	32	LEU	QD2	42440.0
HBP74	35	ILE	HG12	8256.0
QM8	18	HEM	HDM	36216.0
QM8	18	HEM	QM1	13032.0
QM8	32	LEU	QD2	13896.0
QM8	35	ILE	HG12	25432.0
QM8	35	ILE	QD1	8600.0
QM8	59	TRP	HZ2	4806.4
QM8	64	MET	QE	20256.0
QM8	67	TYR	CG	2284.8*2
HDM	18	HEM	QM1	87360.0
QM1	18	HEM	HT2A	1720.8
QM1	18	HEM	QT2	121360.0
QM1	32	LEU	QD1	20080.0
QM1	68	LEU	QD1	73368.0
QM1	68	LEU	QD2	88300.0
QM1	94	LEU	HG	3500.0
QM1	94	LEU	QD2	93040.0
QM1	98	LEU	QD1	55568.0
QM1	98	LEU	QD2	74704.0
HT2A	18	HEM	QT2	96480.0
HT2A	18	HEM	HAM	51568.0
HT2A	18	HEM	QM3	6959.2
HT2A	82	PHE	HZ	2256.0
HT2A	82	PHE	QR	2692.8*5
QT2	18	HEM	HAM	9800.0
QT2	68	LEU	QD1	27744.0
QT2	68	LEU	QD2	83040.0
QT2	82	PHE	HZ	59520.0
QT2	82	PHE	QR	17888.0*5
QT2	85	LEU	HG	16464.0
QT2	85	LEU	QD1	149920.0
QT2	94	LEU	QD1	49400.0
HAM	18	HEM	QM3	18272.0
QM3	18	HEM	HT4A	53704.0
QM3	82	PHE	QR	5572.8*5
HT4A	18	HEM	QT4	71600.0
HT4A	28	VAL	QG1	40992.0
HT4A	81	ALA	QB	60072.0
QT4	28	VAL	QG1	68216.0
HBM	18	HEM	QM5	51360.0
HBM	28	VAL	QG1	25832.0
HBM	81	ALA	HN	16572.0
QM5	18	HEM	HAP61	39968.0
QM5	18	HEM	HAP62	96960.0
QM5	18	HEM	HBP63	30160.0
QM5	18	HEM	HBP64	6287.2
QM5	28	VAL	QG1	118960.0
QM5	29	GLY	HA1	4998.4
QM5	29	GLY	HA2	23112.0
QM5	30	PRO	HD3	27408.0
QM5	46	TYR	HE2	4969.6
QM5	79	LYS+	HG2	19656.0
QM5	79	LYS+	HG3	84160.0
QM5	79	LYS+	HD2	36120.0
QM5	79	LYS+	HE2	13616.0
QM5	79	LYS+	HE3	77368.0
QM5	81	ALA	HN	5645.0
HGM	18	HEM	HAP61	8044.0
HGM	18	HEM	HAP62	21712.0
HGM	18	HEM	HBP64	6097.6
HAP61	18	HEM	HAP62	196240.0
HAP61	18	HEM	HBP63	39080.0
HAP61	30	PRO	HG2	3008.0
HAP61	30	PRO	HD3	8808.0
HAP61	46	TYR	HE2	43480.0
HAP61	48	TYR	CG	17178.0*2
HAP62	18	HEM	HBP63	10760.0
HAP62	18	HEM	HBP64	39620.0
HAP62	29	GLY	HA2	12245.0
HAP62	30	PRO	HB2	1600.0
HAP62	30	PRO	HD2	908.0
HAP62	30	PRO	HD3	9732.0
HAP62	46	TYR	HD1	1392.0
HAP62	46	TYR	HE1	1948.0
HAP62	46	TYR	HE2	44880.0
HAP62	46	TYR	HD2	37664.0
HAP62	48	TYR	CG	5660.0*2
HAP62	79	LYS+	HG3	7012.0
HAP62	79	LYS+	HE2	11976.0
HAP62	79	LYS+	HE3	18812.0
HBP63	18	HEM	HBP64	232160.0
HBP63	78	THR	HG1	5792.4
HBP63	79	LYS+	HG3	119640.0
HBP63	80	MET	HN	15864.0
HBP64	78	THR	HG1	31440.0
HBP64	80	MET	HN	6030.0
19 THR				
HN	19	THR	HA	34008.0
HN	19	THR	QG2	57936.0
HN	31	ASN	HA	46692.0
HN	32	LEU	HN	8689.2
HA	19	THR	HB	195440.0
HA	19	THR	QG2	123200.0
HA	20	VAL	HN	49524.0
HB	19	THR	QG2	228240.0
HB	20	VAL	HN	33552.0
HB	24	GLY	HA1	9328.0
HB	24	GLY	HA2	13200.0
HB	25	PRO	HD2	10528.0
HB	31	ASN	HD21	1368.0
QG2	20	VAL	HN	8023.2
QG2	25	PRO	HD2	29168.0
QG2	27	LYS+	HD2	99840.0
QG2	27	LYS+	HD3	20272.0
QG2	31	ASN	HD21	3566.4
20 VAL				
HN	20	VAL	HA	11196.0
HN	20	VAL	HB	164450.0
HN	20	VAL	QQG	14424.0*2
HN	21	GLU-	HN	3876.0
HA	20	VAL	HB	116240.0
HA	20	VAL	QQG	65120.0*2
HA	32	LEU	HN	78900.0
HA	32	LEU	HB2	21824.0
HA	33	HIS	HN	13296.0
HB	20	VAL	QQG	101220.0*2
QQG	32	LEU	HB2	14508.0*2
QQG	98	LEU	QD1	31424.0*2
QQG	101	ALA	QB	48040.0*2
21 GLU-				
HN	21	GLU-	HA	5113.2
HN	24	GLY	HA2	27216.0
HN	31	ASN	HD21	3416.4
HA	22	LYS+	HN	16980.0
HB2	22	LYS+	HN	11914.8
HB2	24	GLY	HN	20280.0
HB3	22	LYS+	HN	23688.0
22 LYS+				
HN	22	LYS+	HA	22176.0
HA	23	GLY	HN	2509.2
HA	33	HIS	HB2	51216.0
HA	33	HIS	HB3	20040.0
23 GLY				
HN	23	GLY	HA2	7084.8
HA1	24	GLY	HN	4146.0
HA2	24	GLY	HN	44184.0
24 GLY				
HN	24	GLY	HA1	26676.0
HN	24	GLY	HA2	27576.0
HA1	31	ASN	HB2	7216.8

	HA1	31	ASN	HD21	4647.6
	HA2	25	PRO	HD2	239200.0
	HA2	31	ASN	HD21	4783.2
25 PRO					
	HA	25	PRO	HB2	26544.0
	HA	25	PRO	HB3	38748.0
	HA	25	PRO	HG3	26368.0
	HB2	25	PRO	HD2	67912.0
	HB3	25	PRO	HG3	80556.0
26 HIS					
	HA	26	HIS	HB2	77552.0
	HA	26	HIS	HB3	130800.0
	HA	26	HIS	HD2	2412.8
	HA	27	LYS+	HN	80592.0
	HA	30	PRO	HA	66840.0
	HA	31	ASN	HN	59652.0
	HA	31	ASN	HA	3821.6
	HA	31	ASN	HB2	5778.4
	HB2	26	HIS	HD2	57200.0
	HB2	27	LYS+	HN	7478.4
	HB2	46	TYR	HD1	17848.0
	HB3	26	HIS	HD2	31592.0
	HB3	27	LYS+	HN	12348.0
	HB3	30	PRO	HA	41112.0
	HB3	46	TYR	HB2	6327.2
	HB3	46	TYR	HD1	37200.0
	HB3	46	TYR	HE1	50776.0
	HD2	43	ALA	QB	26368.0
	HD2	45	GLY	HA2	47768.0
	HD2	46	TYR	HB2	26880.0
	HD2	46	TYR	HD1	4755.2
	HE1	30	PRO	HA	15024.0
	HE1	30	PRO	HB2	14248.0
	HE1	30	PRO	HB3	18592.0
	HE1	31	ASN	HN	68928.0
	HE1	31	ASN	HA	6955.2
	HE1	31	ASN	HB2	68840.0
	HE1	31	ASN	HB3	30568.0
	HE1	43	ALA	QB	180480.0
	HE1	45	GLY	HA2	3117.6
	HE1	46	TYR	HB2	15280.0
27 LYS+					
	HN	27	LYS+	HB2	5343.6
	HN	31	ASN	HD21	9067.2
	HA	27	LYS+	HB2	5723.2
	HA	27	LYS+	HG3	68376.0
	HB2	27	LYS+	HD2	64200.0
	HB2	28	VAL	HN	15920.0
	HB3	28	VAL	QG2	76716.0
	HG2	27	LYS+	HD2	29128.0
	HG2	27	LYS+	HD3	104720.0
	HG3	27	LYS+	HD2	48072.0
28 VAL					
	HN	28	VAL	HA	6235.0
	HN	28	VAL	HB	29500.0
	HN	28	VAL	QG1	5985.0
	HN	28	VAL	QG2	52050.0
	HA	28	VAL	HB	47472.0
	HA	28	VAL	QG1	135680.0
	HA	28	VAL	QG2	235440.0
	HB	28	VAL	QG1	137840.0
	HB	28	VAL	QG2	343680.0
	QG1	29	GLY	HN	27585.0
29 GLY					
	HN	29	GLY	HA1	22905.0
	HN	29	GLY	HA2	19835.0
	HA1	30	PRO	HD2	3116.0
	HA1	30	PRO	HD3	11744.0
	HA2	30	PRO	HD2	20240.0
	HA2	30	PRO	HD3	38736.0
	HA2	46	TYR	HE2	5062.4
30 PRO					
	HA	30	PRO	HB2	169200.0
	HA	30	PRO	HB3	115440.0
	HA	30	PRO	HG2	20668.0
	HA	30	PRO	HG3	21144.0
	HA	30	PRO	HD2	2129.6
	HA	30	PRO	HD3	11828.0
	HA	31	ASN	HN	363720.0
	HA	31	ASN	HA	4535.2
	HA	46	TYR	HD1	26196.0
	HB2	30	PRO	HG2	94080.0
	HB2	30	PRO	HD2	7368.8
	HB2	30	PRO	HD3	14090.0
	HB2	31	ASN	HN	48540.0
	HB2	46	TYR	HD1	1892.0
	HB2	46	TYR	HE2	4168.0
	HB3	30	PRO	HG2	315900.0
	HB3	30	PRO	HD2	19856.0
	HB3	30	PRO	HD3	77800.0
	HB3	31	ASN	HN	26230.0
	HB3	43	ALA	QB	67840.0
	HB3	46	TYR	HB2	45160.0
	HB3	46	TYR	HD1	15056.0
	HB3	46	TYR	HE1	3366.4
	HB3	46	TYR	HE2	5424.0
	HB3	48	TYR	CG	2626.4*2
	HG2	30	PRO	HD2	17880.0
	HG2	30	PRO	HD3	52920.0
	HG3	30	PRO	HD2	20480.0
	HG3	30	PRO	HD3	47656.0
	HG3	46	TYR	HD1	8452.0
	HG3	46	TYR	HE2	14696.0
	HD3	46	TYR	HD1	4828.0
	HD3	46	TYR	HE1	1528.0
	HD3	46	TYR	HE2	9412.0
	HD3	46	TYR	HD2	7332.0
31 ASN					
	HN	31	ASN	HA	60612.0
	HN	31	ASN	HB2	207240.0
	HN	31	ASN	HB3	99336.0
	HN	32	LEU	HN	1368.0
	HN	43	ALA	QB	11931.6
	HA	31	ASN	HB2	80240.0
	HA	31	ASN	HB3	130000.0
	HA	31	ASN	HD21	25248.0
	HA	32	LEU	HN	223560.0
	HB2	31	ASN	HD21	8283.6
	HB2	31	ASN	HD22	5553.6
32 LEU					
	HN	32	LEU	HB2	32004.0
	HN	32	LEU	HB3	62808.0
	HN	32	LEU	QD2	15100.0
	HN	33	HIS	HN	40740.0
	HA	35	ILE	HB	12780.0
	HB2	35	ILE	QG2	34188.0
	HB2	35	ILE	HG12	24048.0
	HB2	35	ILE	QD1	24112.0
	HB3	35	ILE	HG12	46272.0
	HB3	35	ILE	QD1	4704.0
	QD1	98	LEU	QD1	53080.0
	QD2	35	ILE	HG12	128400.0
33 HIS					
	HN	33	HIS	HA	40200.0
	HN	33	HIS	HB2	88524.0
	HN	33	HIS	HB3	29964.0
	HA	34	GLY	HN	61116.0
34 GLY					
	HN	34	GLY	HA1	22956.0
	HN	34	GLY	HA2	40824.0
	HN	35	ILE	HN	22536.0
	HA1	35	ILE	HN	17196.0
	HA2	35	ILE	HN	6201.6
35 ILE					
	HN	35	ILE	HA	23832.0
	HN	35	ILE	HB	140500.0
	HN	35	ILE	QG2	121400.0
	HN	35	ILE	HG12	21435.0
	HN	35	ILE	QD1	6490.0
	HN	36	PHE	HN	13932.0
	HA	35	ILE	HB	167200.0
	HA	35	ILE	QG2	42720.0
	HA	35	ILE	HG12	298640.0
	HA	35	ILE	QD1	32728.0
	HA	36	PHE	HN	2949.6
	HA	38	ARG+	HN	11869.2
	HA	38	ARG+	HG2	7693.6
	HA	38	ARG+	HD2	131840.0
	HB	35	ILE	QG2	168720.0
	HB	35	ILE	HG12	124200.0
	HB	35	ILE	HG13	55448.0
	HB	35	ILE	QD1	76312.0
	HB	36	PHE	HN	29140.0
	HB	59	TRP	HD1	6757.6

	QG2	35	ILE	HG12	132320.0
	QG2	36	PHE	HN	135150.0
	QG2	36	PHE	CG	13920.0*2
	QG2	36	PHE	CZ	25316.0*2
	QG2	59	TRP	HB3	9816.0
	HG12	35	ILE	QD1	530500.0
	HG12	36	PHE	HA	4652.0
	HG12	59	TRP	HB2	41320.0
	HG12	59	TRP	HD1	183920.0
	HG12	59	TRP	HE1	73450.0
	QD1	36	PHE	HN	15580.0
	QD1	59	TRP	HB3	11448.0
	QD1	59	TRP	HD1	34704.0
36 PHE					
	HN	36	PHE	HA	10700.0
	HN	36	PHE	HB2	56350.0
	HN	36	PHE	CG	13950.0*2
	HN	37	GLY	HN	6303.6
	HA	36	PHE	HB2	46192.0
	HA	36	PHE	HB3	39712.0
	HA	36	PHE	CG	47040.0*2
	HA	36	PHE	CZ	2514.8*2
	HA	37	GLY	HN	117552.0
	HB2	36	PHE	CG	49120.0*2
	HB2	36	PHE	CZ	4472.0*2
	HB2	37	GLY	HN	18120.0
	HB3	36	PHE	CG	34808.0*2
	CG	36	PHE	CZ	37520.0*2*2
	CG	36	PHE	HZ	79240.0*2
	CG	60	ASP-	HA	43240.0*2
	CG	61	GLU-	HN	10932.0*2
	CG	64	MET	QE	5688.0*2
	CG	99	LYS+	HA	35980.0*2
	CG	99	LYS+	HD3	6304.0*2
	CZ	60	ASP-	HA	4264.0*2
	CZ	61	GLU-	HN	2790.6*2
	CZ	61	GLU-	HA	24764.0*2
	CZ	61	GLU-	HB3	37660.0*2
	CZ	64	MET	HB3	19260.0*2
	CZ	64	MET	HG2	49720.0*2
	CZ	98	LEU	HN	740.4*2
	CZ	98	LEU	QD1	4904.0*2
	CZ	99	LYS+	HN	7206.0*2
	CZ	99	LYS+	HA	34476.0*2
	CZ	99	LYS+	HD3	9084.0*2
	HZ	64	MET	QE	122000.0
	HZ	95	ILE	QG2	113920.0
	HZ	95	ILE	HG12	135600.0
	HZ	98	LEU	HB3	92880.0
	HZ	98	LEU	QD1	42640.0
37 GLY					
	HN	37	GLY	HA1	68652.0
	HN	37	GLY	HA2	42084.0
	HN	38	ARG+	HN	80964.0
	HN	58	LEU	QD1	6295.2
	HN	59	TRP	HB2	23892.0
	HA1	38	ARG+	HN	12888.0
	HA1	58	LEU	QD1	6370.8
	HA1	58	LEU	QD2	8546.4
	HA2	38	ARG+	HN	11192.4
38 ARG+					
	HN	38	ARG+	HA	10080.0
	HN	38	ARG+	HB3	31476.0
	HN	38	ARG+	HG2	41510.0
	HN	58	LEU	QD1	15948.0
	HN	59	TRP	HD1	7965.0
	HA	38	ARG+	HB3	21612.0
	HA	38	ARG+	HG2	12732.0
	HA	38	ARG+	HD2	19504.0
	HA	39	HIS	HN	48252.0
	HA	58	LEU	QD1	4920.0
	HB3	39	HIS	HN	40008.0
	HB3	42	GLN	HN	6729.6
	HB3	59	TRP	HD1	6987.2
	HG2	39	HIS	HN	14976.0
	HG2	42	GLN	HB3	133440.0
	HG2	59	TRP	HD1	4745.6
	HD2	42	GLN	HB3	128320.0
	HD2	42	GLN	HG2	31360.0
39 HIS					
	HN	39	HIS	HA	10899.6
	HN	39	HIS	HB2	59208.0
	HN	39	HIS	HB3	23208.0
	HN	42	GLN	HB2	66100.0
	HN	42	GLN	HE21	3553.2
	HN	58	LEU	QD1	5865.6
	HA	39	HIS	HB2	17904.0
	HA	39	HIS	HB3	60024.0
	HA	39	HIS	HD2	18088.0
	HA	40	SER	HN	2707.2
	HA	58	LEU	HA	218400.0
	HA	58	LEU	HB2	13272.0
	HA	58	LEU	QD1	26896.0
	HA	58	LEU	QD2	2710.4
	HB2	39	HIS	HD2	15864.0
	HB2	40	SER	HN	13116.0
	HB2	56	ASN	HA	5879.2
	HB3	39	HIS	HD2	28096.0
	HB3	40	SER	HN	38496.0
	HB3	42	GLN	HE22	9680.0
	HD2	56	ASN	HA	12760.0
	HD2	57	VAL	HA	7988.8
	HD2	58	LEU	HN	8080.0
	HD2	58	LEU	HA	14656.0
	HD2	58	LEU	HB2	18704.0
	HD2	58	LEU	HB3	7704.0
	HD2	58	LEU	QD1	26070.0
	HD2	58	LEU	QD2	4489.6
	HE1	58	LEU	HB2	7662.4
	HE1	58	LEU	QD1	35144.0
	HE1	58	LEU	QD2	11408.0
40 SER					
	HN	40	SER	HA	35988.0
	HN	40	SER	HB2	19488.0
	HN	40	SER	HB3	61992.0
	HN	56	ASN	HA	15576.0
	HN	57	VAL	HN	22704.0
	HN	57	VAL	QG1	8648.4
	HN	57	VAL	QG2	9781.2
	HA	41	GLY	HN	109092.0
	HA	59	TRP	HD1	5014.8
	HA	59	TRP	HE1	208200.0
	HB2	41	GLY	HN	22656.0
	HB2	52	ASN	HD22	2887.2
	HB2	57	VAL	QG2	20152.0
	HB2	59	TRP	HE1	14136.0
	HB2	59	TRP	HZ2	44296.0
	HB3	41	GLY	HN	16548.0
	HB3	52	ASN	HD22	12156.0
	HB3	57	VAL	HN	8728.8
	HB3	57	VAL	QG2	29940.0
	HB3	59	TRP	HE1	38484.0
	HB3	59	TRP	HZ2	45200.0
41 GLY					
	HN	41	GLY	HA1	64560.0
	HN	41	GLY	HA2	37488.0
	HN	42	GLN	HN	22356.0
	HN	52	ASN	HD21	15276.0
	HN	52	ASN	HD22	30900.0
	HN	59	TRP	HD1	6766.8
	HA1	43	ALA	HN	12408.0
	HA1	48	TYR	HB2	25208.0
	HA2	42	GLN	HN	94404.0
	HA2	48	TYR	CG	10176.0*2
	HA2	53	ILE	HA	197280.0
	HA2	53	ILE	QG2	14736.0
	HA2	53	ILE	HG12	48996.0
	HA2	53	ILE	HG13	31968.0
42 GLN					
	HN	42	GLN	HA	17400.0
	HN	42	GLN	HB2	22632.0
	HN	42	GLN	HB3	13995.0
	HN	42	GLN	HG2	15495.0
	HN	42	GLN	HG3	45165.0
	HN	43	ALA	HN	49992.0
	HA	42	GLN	HB2	24416.0
	HA	42	GLN	HB3	71624.0
	HA	42	GLN	HG2	38024.0
	HA	42	GLN	HG3	22120.0
	HB3	42	GLN	HG2	43352.0
	HG2	42	GLN	HE21	5510.0
	HG2	42	GLN	HE22	23715.0
	HG3	42	GLN	HE22	8719.2
43 ALA					

	HN	43	ALA	HA	23904.0
	HN	43	ALA	QB	66228.0
	HA	43	ALA	QB	253280.0
	HA	44	GLU-	HN	148560.0
	QB	44	GLU-	HN	47076.0
44 GLU-					
	HN	44	GLU-	HA	22704.0
	HN	44	GLU-	HB2	206750.0
	HN	44	GLU-	HB3	18648.0
	HN	44	GLU-	HG2	50000.0
	HA	44	GLU-	HB2	184720.0
	HA	44	GLU-	HB3	25320.0
	HA	44	GLU-	HG2	23744.0
46 TYR					
	HN	46	TYR	HA	8362.8
	HN	46	TYR	HB2	22188.0
	HN	46	TYR	HB3	15816.0
	HA	46	TYR	HB2	113600.0
	HA	46	TYR	HB3	43640.0
	HA	46	TYR	HD1	116960.0
	HB2	46	TYR	HD1	38672.0
	HB2	48	TYR	HN	3982.8
	HB2	48	TYR	CG	8160.0*2
	HB3	46	TYR	HD1	15704.0
	HB3	48	TYR	CG	9866.0*2
	HD1	46	TYR	HE1	146240.0
	HD1	46	TYR	HE2	44600.0
	HE2	46	TYR	HD2	267800.0
	HE2	48	TYR	HA	24912.0
	HE2	48	TYR	CG	6658.0*2
	HE2	79	LYS+	HE2	11640.0
	HE2	79	LYS+	HE3	7953.6
	HD2	48	TYR	CG	26280.0*2
47 SER					
	HA	47	SER	HB2	39616.0
	HA	47	SER	HB3	68408.0
48 TYR					
	HN	48	TYR	HA	16200.0
	HN	48	TYR	CG	90625.0*2
	HA	48	TYR	HB2	6411.6
	HA	48	TYR	HB3	75584.0
	HA	48	TYR	CG	10932.0*2
	HA	49	THR	HN	108192.0
	HB2	48	TYR	CG	13996.0*2
	HB2	49	THR	HN	25776.0
	HB2	53	ILE	QG2	21776.0
	HB3	48	TYR	CG	28280.0*2
	HB3	49	THR	HN	74568.0
	HB3	53	ILE	HB	13504.0
	HB3	53	ILE	HG12	33992.0
	HB3	53	ILE	QD1	46936.0
	CG	49	THR	HN	7572.0*2
	CG	52	ASN	HB3	4287.6*2
	CG	52	ASN	HD21	6246.0*2
	CG	52	ASN	HD22	6324.0*2
	CG	53	ILE	HG12	7252.0*2
	CG	53	ILE	QD1	12944.0*2
49 THR					
	HN	49	THR	HA	51372.0
	HN	49	THR	HB	17196.0
	HN	49	THR	QG2	96276.0
	HN	52	ASN	HB3	11440.8
	HN	79	LYS+	HE2	11593.2
	HA	49	THR	HB	145200.0
	HA	49	THR	QG2	169280.0
	HA	50	ASP-	HN	61968.0
	HB	49	THR	QG2	178560.0
	HB	50	ASP-	HN	23316.0
	HB	51	ALA	HN	24048.0
	HB	78	THR	HA	22884.0
	QG2	51	ALA	HN	11844.0
	QG2	78	THR	HA	79544.0
	QG2	79	LYS+	HN	38615.0
	QG2	79	LYS+	HE2	27720.0
50 ASP-					
	HN	50	ASP-	HA	13836.0
	HN	50	ASP-	HB2	15312.0
	HN	50	ASP-	HB3	46296.0
	HN	50	ASP-	QB	53450.0*2
	HN	51	ALA	HN	13185.0
	HA	50	ASP-	HB2	120800.0
	HA	50	ASP-	HB3	66096.0
	HA	51	ALA	HN	5148.0
	HA	53	ILE	HB	124160.0
	HA	53	ILE	QG2	38696.0
	HA	54	LYS+	HN	2388.0
	HA	54	LYS+	HB2	11640.0
	HB2	51	ALA	HN	17675.0
	HB3	51	ALA	HN	15156.0
51 ALA					
	HN	51	ALA	HA	31968.0
	HN	51	ALA	QB	171050.0
	HN	52	ASN	HN	27648.0
	HA	51	ALA	QB	305600.0
	HA	52	ASN	HN	5818.8
	HA	54	LYS+	HN	7905.0
	HA	54	LYS+	HB3	48080.0
	QB	52	ASN	HN	61152.0
	QB	75	ILE	QG2	273760.0
	QB	77	GLY	HA1	44984.0
	QB	78	THR	HN	14148.0
	QB	78	THR	HA	43128.0
	QB	78	THR	HB	23128.0
52 ASN					
	HN	52	ASN	HA	30360.0
	HN	52	ASN	HB2	80340.0
	HN	52	ASN	HB3	46020.0
	HN	53	ILE	HN	54564.0
	HN	75	ILE	QG2	1974.0
	HN	78	THR	HA	4519.2
	HA	52	ASN	HB2	90400.0
	HA	52	ASN	HB3	9560.0
	HA	55	LYS+	HN	12876.0
	HA	55	LYS+	HB3	43784.0
	HA	75	ILE	QG2	112400.0
	HA	75	ILE	QD1	30180.0
	HA	78	THR	HB	3290.4
	HB2	53	ILE	HN	3200.4
	HB2	78	THR	HA	3026.4
	HB2	78	THR	HB	4131.2
	HB3	53	ILE	HN	8973.6
	HB3	53	ILE	HG12	4599.6
	HB3	75	ILE	QG2	29568.0
	HD21	59	TRP	HE1	7460.0
	HD21	75	ILE	QD1	15468.0
53 ILE					
	HN	53	ILE	HA	9016.8
	HN	53	ILE	HB	87900.0
	HN	53	ILE	QG2	45865.0
	HN	53	ILE	HG12	17215.0
	HN	53	ILE	HG13	51000.0
	HN	54	LYS+	HN	64860.0
	HN	55	LYS+	HN	9736.8
	HA	53	ILE	HB	38976.0
	HA	53	ILE	HG12	78456.0
	HA	53	ILE	HG13	35040.0
	HA	53	ILE	QD1	68752.0
	HA	54	LYS+	HN	13608.0
	HB	53	ILE	HG12	84800.0
	HB	53	ILE	QD1	159040.0
	HB	54	LYS+	HN	153350.0
	QG2	53	ILE	HG12	339000.0
	QG2	54	LYS+	HN	71700.0
	QG2	54	LYS+	HA	5908.8
	HG13	53	ILE	QD1	176560.0
	HG13	54	LYS+	HN	16188.0
54 LYS+					
	HN	54	LYS+	HA	32050.0
	HN	54	LYS+	HB2	54792.0
	HN	54	LYS+	HB3	58584.0
	HN	55	LYS+	HN	30645.0
	HA	54	LYS+	HB2	20824.0
	HA	54	LYS+	HB3	120080.0
	HA	55	LYS+	HN	15312.0
	HB2	55	LYS+	HN	8985.0
	HB3	55	LYS+	HN	30020.0
55 LYS+					
	HN	55	LYS+	HA	12950.0
	HN	55	LYS+	HB2	49032.0
	HN	55	LYS+	HB3	43200.0
	HN	55	LYS+	HG2	2338.8
	HA	55	LYS+	HB3	139760.0
	HA	55	LYS+	HG2	62072.0
	HB3	75	ILE	HA	8872.0

	HG2	74 TYR	CG	4272.0*2	
	HG2	74 TYR	CZ	20720.0*2	
56 ASN					
	HN	56 ASN	HA	23196.0	
	HA	56 ASN	HB2	63240.0	
	HA	56 ASN	HB3	72416.0	
57 VAL					
	HN	57 VAL	HA	14076.0	
	HN	57 VAL	HB	47095.0	
	HN	57 VAL	QG1	35832.0	
	HN	57 VAL	QG2	118050.0	
	HN	58 LEU	HN	4065.0	
	HA	57 VAL	HB	111360.0	
	HA	57 VAL	QG1	58648.0	
	HA	57 VAL	QG2	107360.0	
	HA	58 LEU	HN	130800.0	
	HB	57 VAL	QG1	105600.0	
	HB	57 VAL	QG2	212080.0	
	HB	58 LEU	HN	17790.0	
	HB	59 TRP	HZ2	18104.0	
	QG1	58 LEU	HN	67750.0	
	QG1	59 TRP	HA	17312.0	
	QG1	59 TRP	HE3	23970.0	
	QG1	59 TRP	HZ3	7782.4	
	QG1	63 ASN	HD21	33405.0	
	QG1	63 ASN	HD22	32045.0	
	QG1	74 TYR	CZ	23852.0*2	
	QG2	58 LEU	HN	25710.0	
	QG2	74 TYR	CZ	24348.0*2	
	QG2	75 ILE	HG12	9009.6	
	QG2	75 ILE	QD1	19224.0	
58 LEU					
	HN	58 LEU	HA	17100.0	
	HN	58 LEU	HB2	60600.0	
	HN	58 LEU	HG	3435.0	
	HN	58 LEU	QD1	16875.0	
	HN	58 LEU	QD2	8645.0	
	HA	58 LEU	HB2	92160.0	
	HA	58 LEU	QD1	161120.0	
	HA	59 TRP	HN	107376.0	
	HB2	59 TRP	HN	5660.0	
	HB3	58 LEU	QD1	35028.0	
	HB3	58 LEU	QD2	186560.0	
	HG	59 TRP	HN	17550.0	
	QD2	59 TRP	HN	27955.0	
59 TRP					
	HN	59 TRP	HA	12960.0	
	HN	59 TRP	HB2	42564.0	
	HN	59 TRP	HB3	12888.0	
	HN	59 TRP	HD1	5817.6	
	HN	60 ASP-	HN	3117.6	
	HA	59 TRP	HB2	47408.0	
	HA	59 TRP	HB3	150240.0	
	HA	59 TRP	HE3	175120.0	
	HA	59 TRP	HZ3	9440.0	
	HA	60 ASP-	HN	241560.0	
	HA	64 MET	QE	43104.0	
	HB2	59 TRP	HD1	7416.0	
	HB2	59 TRP	HE3	5319.2	
	HB2	64 MET	QE	56408.0	
	HB3	59 TRP	HD1	5161.2	
	HB3	59 TRP	HE3	9616.0	
	HB3	60 ASP-	HN	14976.0	
	HD1	59 TRP	HE1	63504.0	
	HE3	59 TRP	HZ3	127680.0	
	HE3	60 ASP-	HN	50292.0	
	HE3	63 ASN	HB3	1894.4	
	HE3	64 MET	HN	12912.0	
	HE3	64 MET	HA	38832.0	
	HE3	64 MET	HB2	18960.0	
	HE3	64 MET	HB3	20976.0	
	HE3	64 MET	HG2	14944.0	
	HE3	64 MET	QE	84080.0	
	HE1	59 TRP	HZ2	53844.0	
	HZ3	59 TRP	HH2	116880.0	
	HZ3	64 MET	HA	82800.0	
	HZ3	64 MET	HB3	4658.4	
	HZ3	64 MET	HG2	6302.4	
	HZ3	64 MET	QE	15976.0	
	HZ3	67 TYR	HN	7222.8	
	HZ3	67 TYR	HB2	90400.0	
	HZ3	67 TYR	HB3	94080.0	
	HZ3	74 TYR	CZ	19576.0*2	
	HZ2	59 TRP	HH2	163040.0	
	HZ2	67 TYR	HB3	8048.0	
	HZ2	75 ILE	HG13	8232.0	
	HZ2	75 ILE	QD1	69504.0	
	HH2	64 MET	HA	12720.0	
	HH2	67 TYR	HB2	51984.0	
	HH2	67 TYR	HB3	36160.0	
	HH2	74 TYR	CG	12992.0*2	
	HH2	75 ILE	QD1	59192.0	
60 ASP-					
	HN	63 ASN	HN	10298.4	
	HN	63 ASN	HB2	13536.0	
	HN	63 ASN	HB3	4542.0	
	HN	63 ASN	HD21	21456.0	
	HN	63 ASN	HD22	7720.8	
	HN	64 MET	HN	10953.6	
	HN	64 MET	QE	9724.8	
61 GLU-					
	HN	61 GLU-	HA	34380.0	
	HN	61 GLU-	HB2	25764.0	
	HN	61 GLU-	HB3	41640.0	
	HN	61 GLU-	HG2	24684.0	
	HN	62 ASN	HN	34416.0	
	HN	95 ILE	QG2	2347.2	
	HA	61 GLU-	HB2	47696.0	
	HA	61 GLU-	HB3	61096.0	
	HA	61 GLU-	HG2	25716.0	
	HA	62 ASN	HN	6882.0	
	HA	64 MET	HN	1359.6	
	HA	64 MET	HB2	5388.0	
	HA	64 MET	HB3	8936.0	
	HA	64 MET	HG2	43104.0	
	HA	95 ILE	QG2	63984.0	
	HB2	61 GLU-	HG2	146280.0	
	HB2	62 ASN	HN	14016.0	
	HB2	95 ILE	QG2	33432.0	
	HB3	61 GLU-	HG2	247800.0	
	HB3	62 ASN	HN	94550.0	
	HB3	95 ILE	QG2	110232.0	
	HG2	95 ILE	QG2	13680.0	
62 ASN					
	HN	62 ASN	HA	22032.0	
	HN	62 ASN	HB2	21192.0	
	HN	62 ASN	HB3	34510.0	
	HN	63 ASN	HN	88356.0	
	HN	63 ASN	HB3	21192.0	
	HN	64 MET	HN	5187.6	
	HA	62 ASN	HB2	40248.0	
	HA	62 ASN	HB3	34248.0	
	HA	63 ASN	HN	5215.2	
	HA	65 SER	HN	2885.0	
	HA	66 GLU-	HN	1414.8	
	HB2	62 ASN	HD22	59016.0	
	HB2	63 ASN	HN	33048.0	
	HB3	62 ASN	HD21	3350.0	
	HB3	62 ASN	HD22	12984.0	
	HB3	63 ASN	HN	45216.0	
63 ASN					
	HN	63 ASN	HA	49296.0	
	HN	63 ASN	HB2	33984.0	
	HN	63 ASN	HB3	51192.0	
	HN	64 MET	HN	68076.0	
	HN	65 SER	HN	2041.2	
	HA	63 ASN	HB2	122640.0	
	HA	63 ASN	HB3	75904.0	
	HA	64 MET	HN	10908.0	
	HA	66 GLU-	HN	28056.0	
	HA	66 GLU-	HB2	31080.0	
	HB2	63 ASN	HD21	3339.6	
	HB2	63 ASN	HD22	15912.0	
	HB3	63 ASN	HD21	6334.8	
	HB3	63 ASN	HD22	13848.0	
	HB3	64 MET	HN	15696.0	
	HB3	64 MET	HA	14008.0	
64 MET					
	HN	64 MET	HA	45768.0	
	HN	64 MET	HB2	3616.8	
	HN	64 MET	HB3	81576.0	
	HN	64 MET	HG2	17208.0	
	HN	64 MET	QE	22404.0	
	HN	65 SER	HN	23808.0	

	HN	67	TYR	HB2	4156.8
	HA	64	MET	HB3	34640.0
	HA	64	MET	HG2	23312.0
	HA	64	MET	QE	17256.0
	HA	65	SER	HN	13044.0
	HA	67	TYR	HN	6126.0
	HA	67	TYR	HB2	57872.0
	HA	67	TYR	HB3	26368.0
	HA	67	TYR	CG	7986.0*2
	HA	68	LEU	HN	4483.2
	HB2	64	MET	QE	53736.0
	HB3	64	MET	HG2	728320.0
	HB3	64	MET	QE	76688.0
	HB3	95	ILE	QG2	15420.0
	HB3	95	ILE	HG12	30640.0
	HB3	95	ILE	QD1	8184.0
	HG2	64	MET	QE	137280.0
	HG2	65	SER	HN	16960.0
	HG2	68	LEU	HB2	18976.0
	HG2	68	LEU	QD1	22760.0
	HG2	95	ILE	QD1	35152.0
	QE	68	LEU	QD2	43512.0
65 SER					
	HN	65	SER	HA	13135.0
	HN	65	SER	HB2	33264.0
	HN	65	SER	HB3	18576.0
	HN	66	GLU-	HN	30144.0
	HN	67	TYR	HN	10048.8
	HN	95	ILE	QD1	34660.0
	HA	66	GLU-	HN	10149.6
	HA	68	LEU	HN	6438.0
	HA	68	LEU	HB2	11080.0
	HA	68	LEU	QD1	7574.4
	HA	95	ILE	HG13	39528.0
	HA	95	ILE	QD1	65400.0
	HB2	66	GLU-	HN	16452.0
	HB2	95	ILE	QD1	78144.0
	HB3	66	GLU-	HN	32808.0
	HB3	95	ILE	QD1	21152.0
66 GLU-					
	HN	66	GLU-	HA	46305.0
	HN	66	GLU-	HB2	43385.0
	HN	66	GLU-	HB3	56350.0
	HN	66	GLU-	HG2	55300.0
	HN	66	GLU-	HG3	9925.0
	HN	67	TYR	HN	42360.0
	HA	67	TYR	HN	5913.6
	HA	69	THR	HN	6790.8
	HA	69	THR	HB	21544.0
	HA	69	THR	QG2	13608.0
	HB2	67	TYR	HN	38325.0
	HB2	74	TYR	CG	7880.0*2
	HB2	74	TYR	CZ	12904.0*2
	HB3	67	TYR	HN	16245.0
	HG2	74	TYR	CG	2998.2*2
	HG3	74	TYR	CG	16256.0*2
	HG3	74	TYR	CZ	15148.0*2
67 TYR					
	HN	67	TYR	HA	42228.0
	HN	67	TYR	HB2	85344.0
	HN	67	TYR	HB3	81624.0
	HN	67	TYR	HD1	5492.4
	HN	68	LEU	HN	43992.0
	HN	69	THR	HN	4518.0
	HA	67	TYR	HB2	93520.0
	HA	67	TYR	HB3	98160.0
	HA	67	TYR	CG	30320.0*2
	HA	68	LEU	HN	17412.0
	HA	71	PRO	HA	23080.0
	HA	74	TYR	CG	14634.0*2
	HB2	67	TYR	CG	19196.0*2
	HB2	68	LEU	HN	41964.0
	HB2	74	TYR	CG	71560.0*2
	HB3	67	TYR	CG	7940.0*2
	HB3	74	TYR	CG	16876.0*2
	CG	68	LEU	HN	3382.5*2
	CG	68	LEU	HG	7488.0*2
	CG	68	LEU	QD1	2213.2*2
	CG	68	LEU	QD2	5956.0*2
	CG	71	PRO	HA	8644.0*2
	CG	74	TYR	HB2	9324.0*2
	CG	74	TYR	HB3	29464.0*2
	CG	74	TYR	CG	15638.0*2*2
	CG	75	ILE	QD1	8244.0*2
	CZ	68	LEU	QD2	3976.8*2
	CZ	71	PRO	HB2	4536.0*2
	CZ	74	TYR	HB3	6520.0*2
	CZ	75	ILE	HN	3852.5*2
	CZ	75	ILE	HG13	3364.0*2
	CZ	75	ILE	QD1	3144.0*2
68 LEU					
	HN	68	LEU	HA	30108.0
	HN	68	LEU	HB2	72750.0
	HN	68	LEU	HB3	29605.0
	HN	68	LEU	HG	112900.0
	HN	68	LEU	QD1	44000.0
	HN	68	LEU	QD2	44350.0
	HN	69	THR	HN	35390.0
	HA	68	LEU	HB2	85840.0
	HA	68	LEU	HB3	66680.0
	HA	68	LEU	HG	21208.0
	HA	68	LEU	QD1	12848.0
	HA	68	LEU	QD2	176920.0
	HA	69	THR	HN	2626.8
	HA	71	PRO	HG2	45248.0
	HA	71	PRO	HD3	9471.6
	HA	84	GLY	HA1	9728.0
	HB2	68	LEU	HG	61800.0
	HB2	68	LEU	QD1	104800.0
	HB2	68	LEU	QD2	53504.0
	HB2	69	THR	HN	16835.0
	HB2	85	LEU	HB2	27920.0
	HB3	68	LEU	HG	57468.0
	HB3	68	LEU	QD1	90080.0
	HB3	68	LEU	QD2	56288.0
	HB3	82	PHE	QR	862.1*5
	HB3	85	LEU	HN	5980.8
	HG	68	LEU	QD1	145840.0
	HG	68	LEU	QD2	105120.0
	QD1	82	PHE	QR	512.5*5
	QD1	94	LEU	QD2	87040.0
	QD1	95	ILE	HG12	68536.0
	QD1	95	ILE	QD1	61524.0
	QD2	69	THR	HN	15375.0
	QD2	71	PRO	HA	4116.0
	QD2	71	PRO	HD3	10976.0
	QD2	82	PHE	HZ	7012.0
	QD2	82	PHE	QR	4995.2*5
	QD2	94	LEU	QD2	42688.0
	QD2	95	ILE	HG12	3281.6
	QD2	95	ILE	QD1	11488.0
	QD2	98	LEU	QD1	16072.0
69 THR					
	HN	69	THR	HA	25500.0
	HN	69	THR	HB	22656.0
	HN	69	THR	QG2	13965.0
	HN	70	ASN	HN	39492.0
	HN	82	PHE	QR	1370.4*5
	HA	69	THR	HB	26280.0
	HA	69	THR	QG2	20064.0
	HA	70	ASN	HN	4844.4
	HA	70	ASN	HB2	4249.6
	HA	85	LEU	HN	28872.0
	HB	69	THR	QG2	88116.0
	HB	70	ASN	HN	10978.8
	HB	70	ASN	HB3	22512.0
	QG2	70	ASN	HN	3365.0
	QG2	70	ASN	HB2	25044.0
	QG2	86	LYS+	HA	6517.2
70 ASN					
	HN	70	ASN	HA	13968.0
	HN	70	ASN	HB2	6558.0
	HN	71	PRO	HD3	4770.0
	HA	70	ASN	HB2	68576.0
	HA	70	ASN	HB3	51400.0
	HA	71	PRO	HD2	28352.0
	HA	71	PRO	HD3	208720.0
	HA	72	TML	HN	21120.0
	HA	73	LYS+	HN	3697.2
	HA	73	LYS+	HB3	6858.0
	HA	84	GLY	HA1	11056.0
	HA	84	GLY	HA2	44248.0
	HB2	73	LYS+	HB2	13824.0
71 PRO					

	HA	71	PRO	HB2	100560.0
	HA	71	PRO	HG3	11840.0
	HA	71	PRO	HD2	59176.0
	HA	72	TML	HN	29520.0
	HA	74	TYR	HN	6879.6
	HA	74	TYR	HB2	50808.0
	HA	74	TYR	HB3	11232.0
	HA	74	TYR	CG	4636.0*2
	HA	75	ILE	HN	14316.0
	HA	78	THR	QG2	18256.0
	HB2	72	TML	HN	93096.0
	HB2	78	THR	QG2	19528.0
	HB3	71	PRO	HG3	5964.8
	HB3	78	THR	QG2	13960.0
	HG2	78	THR	QG2	45924.0
	HG2	82	PHE	QR	8152.0*5
	HG3	71	PRO	HD3	350400.0
	HG3	82	PHE	QR	9857.6*5
	HD2	82	PHE	QR	7752.0*5
	HD2	84	GLY	HA1	49464.0
	HD2	85	LEU	HN	4422.0
	HD3	72	TML	HN	14328.0
	HD3	82	PHE	QR	20416.0*5
	HD3	84	GLY	HA1	102880.0
	HD3	84	GLY	HA2	81200.0
72 TML					
	HN	72	TML	HA	62184.0
	HN	72	TML	HB2	173400.0
	HN	72	TML	HG3	7137.6
	HN	73	LYS+	HN	53940.0
	HA	72	TML	HB2	235440.0
	HA	72	TML	HG2	61320.0
	HA	72	TML	HG3	85880.0
	HA	72	TML	HE2	7360.0
	HA	73	LYS+	HN	5533.2
	HA	75	ILE	HN	32436.0
	HA	75	ILE	HB	10536.0
	HA	77	GLY	HN	9903.6
	HA	78	THR	QG2	161160.0
	HB2	72	TML	HE2	22648.0
	HB2	72	TML	QQH	15736.0
	HB2	73	LYS+	HN	19020.0
	HB2	78	THR	QG2	78840.0
	HG2	78	THR	QG2	85760.0
	HG3	78	THR	QG2	55200.0
	HE2	81	ALA	HA	89880.0
	QQH	81	ALA	HA	28432.0
73 LYS+					
	HN	73	LYS+	HA	33624.0
	HN	73	LYS+	HB2	34656.0
	HN	73	LYS+	HB3	139800.0
	HN	74	TYR	HN	99204.0
	HN	75	ILE	HN	17832.0
	HA	73	LYS+	HD2	14848.0
	HA	74	TYR	HN	23112.0
	HA	76	PRO	HG3	6198.0
	HB2	74	TYR	HN	9127.2
	HB3	74	TYR	HN	21852.0
74 TYR					
	HN	74	TYR	HB2	79212.0
	HN	74	TYR	HB3	42768.0
	HN	74	TYR	CG	7260.0*2
	HN	75	ILE	HN	123480.0
	HA	74	TYR	HB2	82720.0
	HA	74	TYR	HB3	35320.0
	HA	74	TYR	CG	17316.0*2
	HA	75	ILE	HN	6783.6
	HB2	74	TYR	CG	45120.0*2
	HB2	75	ILE	HN	36648.0
	HB2	75	ILE	HG13	63336.0
	HB3	74	TYR	CG	77120.0*2
	HB3	75	ILE	HN	52608.0
	CG	74	TYR	CZ	70520.0*2*2
	CG	75	ILE	HN	5186.4*2
	CG	75	ILE	HB	4736.0*2
	CG	75	ILE	QG2	1908.0*2
	CG	75	ILE	HG12	27484.0*2
	CG	75	ILE	QD1	66240.0*2
	CZ	75	ILE	HG12	3230.8*2
	CZ	75	ILE	HG13	10158.0*2
	CZ	75	ILE	QD1	15690.0*2
75 ILE					
	HN	75	ILE	HA	46596.0
	HN	75	ILE	HB	15425.0
	HN	75	ILE	QG2	1329.6
	HN	75	ILE	HG12	3794.4
	HN	75	ILE	HG13	32412.0
	HN	78	THR	QG2	5115.6
	HA	75	ILE	HB	49328.0
	HA	75	ILE	QG2	63440.0
	HA	75	ILE	HG12	29496.0
	HA	75	ILE	HG13	23456.0
	HA	75	ILE	QD1	15240.0
	HA	76	PRO	HG3	4619.2
	HA	76	PRO	HD3	100800.0
	HB	75	ILE	QG2	81156.0
	HB	75	ILE	HG12	11503.2
	HB	78	THR	HN	19176.0
	HB	78	THR	HB	104960.0
	QG2	75	ILE	QD1	223360.0
	QG2	76	PRO	HD3	32580.0
	QG2	78	THR	HN	20700.0
	QG2	78	THR	HA	27568.0
	QG2	78	THR	HB	113520.0
	HG12	75	ILE	QD1	36888.0
	HG13	75	ILE	QD1	69204.0
	HG13	78	THR	QG2	15036.0
	QD1	78	THR	HB	18520.0
76 PRO					
	HA	76	PRO	HB2	53256.0
	HA	76	PRO	HB3	112320.0
	HA	76	PRO	HG3	47976.0
	HA	77	GLY	HN	11953.2
	HA	78	THR	HN	5841.6
	HB3	76	PRO	HG3	38700.0
	HB3	76	PRO	HD3	9780.0
	HG3	76	PRO	HD3	26340.0
77 GLY					
	HN	78	THR	HN	29880.0
	HA1	78	THR	HN	13548.0
	HA2	78	THR	HN	10958.4
78 THR					
	HN	78	THR	HA	56472.0
	HN	78	THR	HB	93612.0
	HN	78	THR	QG2	137520.0
	HA	78	THR	HB	175200.0
	HA	78	THR	QG2	132800.0
	HA	78	THR	HG1	41784.0
	HA	79	LYS+	HN	27780.0
	HA	80	MET	HN	9243.6
	HB	78	THR	QG2	222480.0
	HB	78	THR	HG1	35064.0
	HB	79	LYS+	HN	6112.8
	QG2	78	THR	HG1	3250.8
	QG2	80	MET	HN	19656.0
	HG1	79	LYS+	HN	30720.0
	HG1	80	MET	HN	27708.0
79 LYS+					
	HN	79	LYS+	HA	19632.0
	HN	79	LYS+	HB3	11185.0
	HN	79	LYS+	HG2	12552.0
	HN	79	LYS+	HG3	26810.0
	HN	80	MET	HN	38796.0
	HA	79	LYS+	HB2	104800.0
	HA	79	LYS+	HB3	124320.0
	HA	79	LYS+	HG2	33216.0
	HA	79	LYS+	HG3	6294.4
	HA	79	LYS+	HD2	22128.0
	HA	80	MET	HN	13416.0
	HB2	79	LYS+	HG2	218400.0
	HB2	80	MET	HN	5710.8
	HB3	79	LYS+	HG2	115360.0
	HB3	79	LYS+	HG3	7875.2
	HB3	80	MET	HN	2863.2
	HG2	79	LYS+	HE3	156000.0
	HG3	79	LYS+	HD2	169280.0
	HG3	79	LYS+	HE2	29776.0
	HG3	79	LYS+	HE3	56896.0
	HG3	80	MET	HN	10339.2
	HD2	79	LYS+	HE2	88560.0
	HD2	79	LYS+	HE3	94240.0
81 ALA					
	HN	81	ALA	HA	19932.0
	HN	81	ALA	QB	141700.0

	HN	82	PHE	HN	12120.0
	HA	81	ALA	QB	251120.0
	HA	82	PHE	HN	135240.0
82 PHE					
	HN	82	PHE	HB2	8684.4
	HB2	82	PHE	QR	6043.2*5
	HB2	85	LEU	QD2	7197.6
	HB3	82	PHE	QR	20400.0*5
	HE1	85	LEU	HN	38208.0
	HE1	85	LEU	QD1	18870.0
	HE1	85	LEU	QD2	12540.0
	HZ	82	PHE	QR	76496.0*5
	HZ	84	GLY	HA2	6320.0
	HZ	85	LEU	HA	6860.0
	HZ	85	LEU	HG	90080.0
	HZ	85	LEU	QD1	33152.0
	HZ	85	LEU	QD2	80480.0
	QR	84	GLY	HA1	10041.6*5
	QR	85	LEU	HG	22304.0*5
	QR	85	LEU	QD1	7468.8*5
	QR	85	LEU	QD2	5123.2*5
84 GLY					
	HA1	85	LEU	HN	78696.0
	HA1	85	LEU	HG	6520.8
	HA2	85	LEU	HN	78924.0
85 LEU					
	HN	85	LEU	HA	9331.2
	HN	85	LEU	HB2	44545.0
	HN	85	LEU	HB3	12564.0
	HN	85	LEU	HG	15515.0
	HN	85	LEU	QD1	94700.0
	HA	85	LEU	HB3	62632.0
	HA	85	LEU	QD1	15744.0
	HA	85	LEU	QD2	138000.0
	HB2	85	LEU	QD1	68776.0
	HB2	91	ARG+	HN	3776.4
	HB3	85	LEU	QD1	76208.0
	HB3	85	LEU	QD2	27616.0
	HG	85	LEU	QD1	117920.0
	QD1	90	ASP-	HB2	8592.0
	QD1	90	ASP-	HB3	1979.2
	QD1	91	ARG+	HA	20808.0
	QD2	90	ASP-	HB2	42856.0
	QD2	90	ASP-	HB3	3495.2
86 LYS+					
	HN	86	LYS+	HA	3841.2
	HN	86	LYS+	HB3	26448.0
	HA	86	LYS+	HB2	48888.0
	HA	86	LYS+	HB3	195920.0
	HA	86	LYS+	HG2	17432.0
	HA	87	LYS+	HN	4011.6
	HB3	87	LYS+	HN	31505.0
87 LYS+					
	HN	87	LYS+	HA	12732.0
	HN	87	LYS+	HB2	177650.0
	HN	87	LYS+	HB3	40215.0
	HN	90	ASP-	HB3	3697.2
	HB2	90	ASP-	HN	62600.0
	HB3	88	GLU-	HN	34068.0
	HB3	90	ASP-	HB2	22572.0
	HB3	90	ASP-	HB3	11162.4
88 GLU-					
	HN	88	GLU-	HA	23040.0
	HA	88	GLU-	HB2	26136.0
	HA	91	ARG+	HB2	14172.0
	HB3	89	LYS+	HN	33075.0
89 LYS+					
	HN	89	LYS+	HA	11095.0
	HN	89	LYS+	HB2	83600.0
	HN	89	LYS+	HB3	97550.0
	HN	90	ASP-	HN	17755.0
	HN	92	ASN	HD21	1260.0
	HA	89	LYS+	HB3	143920.0
	HA	92	ASN	HB2	46744.0
	HB2	90	ASP-	HN	48300.0
90 ASP-					
	HN	90	ASP-	HB2	19115.0
	HN	90	ASP-	HB3	35135.0
	HN	91	ARG+	HN	22044.0
	HN	92	ASN	HN	1258.8
	HA	90	ASP-	HB2	98400.0
	HA	90	ASP-	HB3	84880.0
	HA	93	ASP-	HB3	10066.8
	HB3	91	ARG+	HN	10876.8
91 ARG+					
	HN	91	ARG+	HA	13255.0
	HN	91	ARG+	HB2	20904.0
	HN	92	ASN	HN	53196.0
	HA	91	ARG+	HB2	16380.0
	HA	92	ASN	HN	4095.6
	HA	94	LEU	HN	33276.0
	HA	94	LEU	HB2	22656.0
	HA	94	LEU	HB3	58344.0
	HB2	92	ASN	HN	30000.0
92 ASN					
	HN	92	ASN	HA	21780.0
	HN	92	ASN	HB2	54108.0
	HN	92	ASN	HB3	48576.0
	HN	92	ASN	HD21	1382.4
	HA	93	ASP-	HN	6080.0
	HA	95	ILE	HN	4716.0
93 ASP-					
	HN	93	ASP-	HA	47136.0
	HN	93	ASP-	HB2	100548.0
	HN	93	ASP-	HB3	28780.0
	HN	94	LEU	HN	52716.0
	HA	93	ASP-	HB3	91520.0
	HA	94	LEU	HN	2470.8
	HB3	94	LEU	HN	33984.0
94 LEU					
	HN	94	LEU	HA	17136.0
	HN	94	LEU	HB2	116736.0
	HN	94	LEU	HB3	18024.0
	HN	94	LEU	HG	7630.8
	HN	94	LEU	QD2	27310.0
	HN	95	ILE	HN	36450.0
	HA	94	LEU	HG	40472.0
	HA	94	LEU	QD2	23744.0
	HA	95	ILE	HN	21756.0
	HA	97	TYR	HN	10012.8
	HA	98	LEU	HG	12424.0
	HB2	94	LEU	QD2	69552.0
	HB2	95	ILE	HN	22668.0
	HB3	94	LEU	HG	13572.0
	HB3	94	LEU	QD2	23772.0
	HB3	95	ILE	HN	114240.0
	HG	94	LEU	QD1	47184.0
	HG	94	LEU	QD2	71928.0
	HG	95	ILE	HN	8675.0
	HG	98	LEU	HB3	24160.0
	HG	98	LEU	HG	101040.0
	HG	98	LEU	QD1	93040.0
	QD2	95	ILE	HN	5704.8
95 ILE					
	HN	95	ILE	HA	28956.0
	HN	95	ILE	HB	60024.0
	HN	95	ILE	QG2	46716.0
	HN	95	ILE	HG13	17700.0
	HN	95	ILE	QD1	22728.0
	HN	96	THR	HN	49932.0
	HA	95	ILE	HB	51424.0
	HA	95	ILE	QG2	130640.0
	HA	95	ILE	QD1	4176.8
	HA	98	LEU	HN	28416.0
	HA	98	LEU	HB2	98400.0
	HA	98	LEU	QD2	19408.0
	HB	95	ILE	QG2	158240.0
	HB	95	ILE	HG13	20736.0
	HB	95	ILE	QD1	112720.0
	HB	96	THR	HN	9444.0
	QG2	95	ILE	HG12	297520.0
	QG2	95	ILE	QD1	299760.0
	QG2	96	THR	HN	9490.0
	QG2	96	THR	HA	20184.0
	QG2	99	LYS+	HN	3163.2
	HG12	95	ILE	QD1	72360.0
	HG13	95	ILE	QD1	92232.0
96 THR					
	HN	96	THR	HA	16248.0
	HN	96	THR	HB	31668.0
	HN	96	THR	QG2	9865.0
	HN	97	TYR	HN	32880.0
	HN	98	LEU	HN	3787.2
	HA	96	THR	HB	195280.0

	HA	96	THR	QG2	191680.0
	HA	99	LYS+	HN	9575.0
	HA	99	LYS+	HB2	7380.0
	HA	99	LYS+	HG2	13792.0
	HA	99	LYS+	HD2	12184.0
	HB	96	THR	QG2	85920.0
	HB	97	TYR	HN	18948.0
	QG2	97	TYR	HN	19680.0
97 TYR					
	HN	97	TYR	HA	56376.0
	HN	97	TYR	HB2	16932.0
	HN	97	TYR	HB3	35400.0
	HN	98	LEU	HN	35292.0
	HA	98	LEU	HN	15252.0
	HA	100	LYS+	HB2	41640.0
	HB2	98	LEU	HN	23328.0
	HB3	98	LEU	HN	25368.0
	HD1	97	TYR	HE1	8856.0
	HD2	98	LEU	HG	6872.8
98 LEU					
	HN	98	LEU	HA	38580.0
	HN	98	LEU	HB2	59424.0
	HN	98	LEU	HB3	17630.0
	HN	98	LEU	HG	82716.0
	HN	98	LEU	QD1	15775.0
	HN	98	LEU	QD2	27775.0
	HN	99	LYS+	HN	44352.0
	HA	98	LEU	HB2	186080.0
	HA	98	LEU	HG	36784.0
	HA	98	LEU	QD1	29576.0
	HA	98	LEU	QD2	147120.0
	HA	99	LYS+	HN	9384.0
	HA	101	ALA	HN	23784.0
	HA	101	ALA	QB	104160.0
	HB2	98	LEU	QD1	57228.0
	HB2	98	LEU	QD2	96720.0
	HB2	99	LYS+	HN	48516.0
	HB3	98	LEU	QD1	52672.0
	HB3	98	LEU	QD2	83200.0
	HG	98	LEU	QD1	98560.0
	HG	98	LEU	QD2	96240.0
	QD2	102	SER	HN	8880.0
99 LYS+					
	HN	99	LYS+	HA	45865.0
	HN	99	LYS+	HB2	127450.0
	HN	99	LYS+	HB3	78384.0
	HN	99	LYS+	HG2	25905.0
	HN	99	LYS+	HD3	52750.0
	HN	100	LYS+	HN	39552.0
	HN	101	ALA	HN	8042.4
	HA	99	LYS+	HB2	75392.0
	HA	99	LYS+	HB3	20076.0
	HA	99	LYS+	HG2	62744.0
	HA	99	LYS+	HD2	72808.0
	HA	99	LYS+	HD3	38512.0
	HB2	100	LYS+	HN	34550.0
	HB3	100	LYS+	HN	6453.6
100 LYS+					
	HN	100	LYS+	HA	29490.0
	HN	100	LYS+	HB2	180200.0
	HN	100	LYS+	HB3	107900.0
	HN	101	ALA	HN	77124.0
	HA	100	LYS+	HB2	173440.0
	HA	101	ALA	HN	12876.0
	HA	103	GLU-	HB2	21984.0
	HB2	101	ALA	HN	77750.0
	HB3	101	ALA	HN	27625.0
101 ALA					
	HN	101	ALA	HA	54060.0
	HN	101	ALA	QB	239850.0
	HN	102	SER	HN	60200.0
	HA	101	ALA	QB	235600.0
	QB	102	SER	HN	54000.0
102 SER					
	HN	102	SER	HB2	17580.0
	HN	103	GLU-	HN	79860.0
	HB2	103	GLU-	HN	16092.0
103 GLU-					
	HN	103	GLU-	HA	19080.0
	HN	103	GLU-	HB2	178400.0
	HN	103	GLU-	HB3	25555.0

1D NOE constraints

18 HEM					
	QM3	80	MET	QE	6.0
	HA	18	HEM	HD1	4.0
	HB2	18	HEM	HD1	4.0
	HB3	18	HEM	HD1	4.0
68 LEU					
	QD2	80	MET	QE	6.0

Irrelevant NOE constraints

HN	PHE	-3	- HB2	PHE	-3
HA	PHE	-3	- CG	PHE	-3
HA	PHE	-3	- HN	LYS+	-2
HB2	PHE	-3	- CG	PHE	-3
HB3	PHE	-3	- CG	PHE	-3
CG	PHE	-3	- CZ	PHE	-3
CZ	PHE	-3	- HZ	PHE	-3
HN	LYS+	-2	- HA	LYS+	-2
HA	LYS+	-2	- HB2	LYS+	-2
HA	LYS+	-2	- HN	ALA	-1
HN	ALA	-1	- HA	ALA	-1
HA	ALA	-1	- QB	ALA	-1
HA	ALA	-1	- HN	GLY	1
HN	GLY	1	- HA1	GLY	1
HA2	GLY	1	- HN	SER	2
HN	SER	2	- HA	SER	2
HN	SER	2	- HB2	SER	2
HN	SER	2	- HB3	SER	2
HN	ALA	3	- HA	ALA	3
HN	ALA	3	- QB	ALA	3
HA	ALA	3	- QB	ALA	3
HN	LYS+	5	- HA	LYS+	5
HA	LYS+	5	- HN	GLY	6
HN	GLY	6	- HA1	GLY	6
HN	GLY	6	- HA2	GLY	6
HA2	GLY	6	- HN	ALA	7
HN	ALA	7	- HA	ALA	7
HA	ALA	7	- QB	ALA	7
HA	ALA	7	- HN	THR	8
HN	THR	8	- HA	THR	8
HA	THR	8	- QG2	THR	8
HA	THR	8	- HN	LEU	9
HB	THR	8	- QG2	THR	8
HN	LEU	9	- HA	LEU	9
HA	LEU	9	- HB3	LEU	9
HA	LEU	9	- HN	PHE	10
HB3	LEU	9	- QD1	LEU	9
HG	LEU	9	- QD1	LEU	9
HG	LEU	9	- QD2	LEU	9
HN	PHE	10	- HA	PHE	10
HA	PHE	10	- HB2	PHE	10
HA	PHE	10	- HB3	PHE	10
HA	PHE	10	- CG	PHE	10
HA	PHE	10	- HN	LYS+	11
HB2	PHE	10	- CG	PHE	10
HB3	PHE	10	- CG	PHE	10
CG	PHE	10	- CZ	PHE	10
CG	PHE	10	- HZ	PHE	10
CZ	PHE	10	- HZ	PHE	10
HN	LYS+	11	- HA	LYS+	11
HA	LYS+	11	- HB2	LYS+	11
HA	LYS+	11	- HB3	LYS+	11
HA	LYS+	11	- HN	THR	12
HB2	LYS+	11	- HG2	LYS+	11
HN	THR	12	- HA	THR	12
HA	THR	12	- HB	THR	12
HA	THR	12	- QG2	THR	12
HA	THR	12	- HN	ARG+	13
HB	THR	12	- QG2	THR	12
HN	ARG+	13	- HA	ARG+	13
HA	ARG+	13	- HB2	ARG+	13
HA	ARG+	13	- HB3	ARG+	13
HA	ARG+	13	- HN	CYSS	14
HN	CYSS	14	- HA	CYSS	14
HA	CYSS	14	- HN	LEU	15
HN	LEU	15	- HA	LEU	15
HA	LEU	15	- HB3	LEU	15
HB2	LEU	15	- QD2	LEU	15
HB3	LEU	15	- QD2	LEU	15

HG	LEU	15 -	QD1	LEU	15
HG	LEU	15 -	QD2	LEU	15
HG3	GLN	16 -	HE21	GLN	16
HN	CYSS	17 -	HA	CYSS	17
HN	CYSS	17 -	HB2	CYSS	17
HA	CYSS	17 -	HB2	CYSS	17
HA	CYSS	17 -	HB3	CYSS	17
HA	CYSS	17 -	HN	HEM	18
HN	HEM	18 -	HA	HEM	18
HN	HEM	18 -	HB3	HEM	18
HA	HEM	18 -	HB3	HEM	18
HB2	HEM	18 -	HD1	HEM	18
HB3	HEM	18 -	HD1	HEM	18
HAP71	HEM	18 -	HAP72	HEM	18
HAP71	HEM	18 -	HBP73	HEM	18
HAP71	HEM	18 -	HBP74	HEM	18
HAP72	HEM	18 -	HBP73	HEM	18
HAP72	HEM	18 -	HBP74	HEM	18
HAP72	HEM	18 -	HGM	HEM	18
HBP73	HEM	18 -	HBP74	HEM	18
QM8	HEM	18 -	HDM	HEM	18
HDM	HEM	18 -	QM1	HEM	18
HT2A	HEM	18 -	QT2	HEM	18
HAM	HEM	18 -	QM3	HEM	18
HT4A	HEM	18 -	QT4	HEM	18
HBM	HEM	18 -	QM5	HEM	18
HGM	HEM	18 -	HAP61	HEM	18
HAP61	HEM	18 -	HAP62	HEM	18
HAP61	HEM	18 -	HBP63	HEM	18
HAP62	HEM	18 -	HBP63	HEM	18
HAP62	HEM	18 -	HBP64	HEM	18
HBP63	HEM	18 -	HBP64	HEM	18
HN	THR	19 -	HA	THR	19
HA	THR	19 -	QG2	THR	19
HB	THR	19 -	QG2	THR	19
HN	VAL	20 -	HA	VAL	20
HN	VAL	20 -	QQG	VAL	20
HA	VAL	20 -	QQG	VAL	20
HB	VAL	20 -	QQG	VAL	20
HN	GLU-	21 -	HA	GLU-	21
HA	GLU-	21 -	HN	LYS+	22
HN	LYS+	22 -	HA	LYS+	22
HA	LYS+	22 -	HN	GLY	23
HN	GLY	23 -	HA2	GLY	23
HA1	GLY	23 -	HN	GLY	24
HN	GLY	24 -	HA1	GLY	24
HN	GLY	24 -	HA2	GLY	24
HA	PRO	25 -	HB2	PRO	25
HA	PRO	25 -	HB3	PRO	25
HA	PRO	25 -	HG3	PRO	25
HB2	PRO	25 -	HD2	PRO	25
HB3	PRO	25 -	HG3	PRO	25
HA	HIS	26 -	HB2	HIS	26
HN	LYS+	27 -	HB2	LYS+	27
HA	LYS+	27 -	HB2	LYS+	27
HG2	LYS+	27 -	HD2	LYS+	27
HG3	LYS+	27 -	HD2	LYS+	27
HN	VAL	28 -	HA	VAL	28
HN	VAL	28 -	QG1	VAL	28
HA	VAL	28 -	HB	VAL	28
HA	VAL	28 -	QG1	VAL	28
HB	VAL	28 -	QG1	VAL	28
HB	VAL	28 -	QG2	VAL	28
HN	GLY	29 -	HA1	GLY	29
HN	GLY	29 -	HA2	GLY	29
HA1	GLY	29 -	HD2	PRO	30
HA1	GLY	29 -	HD3	PRO	30
HA	PRO	30 -	HB2	PRO	30
HA	PRO	30 -	HB3	PRO	30
HA	PRO	30 -	HG2	PRO	30
HA	PRO	30 -	HG3	PRO	30
HA	PRO	30 -	HD2	PRO	30
HA	PRO	30 -	HD3	PRO	30
HB2	PRO	30 -	HG2	PRO	30
HB2	PRO	30 -	HD2	PRO	30
HB2	PRO	30 -	HD3	PRO	30
HB3	PRO	30 -	HG2	PRO	30
HB3	PRO	30 -	HD2	PRO	30
HB3	PRO	30 -	HD3	PRO	30
HG2	PRO	30 -	HD2	PRO	30
HG2	PRO	30 -	HD3	PRO	30
HG3	PRO	30 -	HD2	PRO	30
HG3	PRO	30 -	HD3	PRO	30
HN	ASN	31 -	HA	ASN	31
HA	ASN	31 -	HB2	ASN	31
HB2	ASN	31 -	HD21	ASN	31
HB2	ASN	31 -	HD22	ASN	31
HN	HIS	33 -	HA	HIS	33
HN	GLY	34 -	HA1	GLY	34
HN	GLY	34 -	HA2	GLY	34
HA1	GLY	34 -	HN	ILE	35
HA2	GLY	34 -	HN	ILE	35
HN	ILE	35 -	HA	ILE	35
HA	ILE	35 -	QG2	ILE	35
HA	ILE	35 -	QD1	ILE	35
HA	ILE	35 -	HN	PHE	36
HB	ILE	35 -	QG2	ILE	35
HB	ILE	35 -	QD1	ILE	35
QG2	ILE	35 -	HG12	ILE	35
HG12	ILE	35 -	QD1	ILE	35
HN	PHE	36 -	HA	PHE	36
HN	PHE	36 -	CG	PHE	36
HA	PHE	36 -	HB2	PHE	36
HA	PHE	36 -	HB3	PHE	36
HA	PHE	36 -	CG	PHE	36
HB2	PHE	36 -	CG	PHE	36
HB2	PHE	36 -	CZ	PHE	36
HB3	PHE	36 -	CG	PHE	36
CG	PHE	36 -	CZ	PHE	36
CG	PHE	36 -	HZ	PHE	36
HN	GLY	37 -	HA1	GLY	37
HN	GLY	37 -	HA2	GLY	37
HA1	GLY	37 -	HN	ARG+	38
HA2	GLY	37 -	HN	ARG+	38
HN	ARG+	38 -	HA	ARG+	38
HA	ARG+	38 -	HB3	ARG+	38
HN	HIS	39 -	HA	HIS	39
HA	HIS	39 -	HB2	HIS	39
HA	HIS	39 -	HB3	HIS	39
HA	HIS	39 -	HN	SER	40
HN	SER	40 -	HA	SER	40
HN	GLY	41 -	HA1	GLY	41
HN	GLY	41 -	HA2	GLY	41
HN	GLN	42 -	HA	GLN	42
HA	GLN	42 -	HB2	GLN	42
HA	GLN	42 -	HB3	GLN	42
HB3	GLN	42 -	HG2	GLN	42
HG2	GLN	42 -	HE21	GLN	42
HG3	GLN	42 -	HE22	GLN	42
HN	ALA	43 -	HA	ALA	43
HA	ALA	43 -	QB	ALA	43
HN	GLU-	44 -	HA	GLU-	44
HA	GLU-	44 -	HB3	GLU-	44
HN	TYR	46 -	HA	TYR	46
HA	TYR	46 -	HB3	TYR	46
HB3	TYR	46 -	HD1	TYR	46
HD1	TYR	46 -	HE1	TYR	46
HD1	TYR	46 -	HE2	TYR	46
HE2	TYR	46 -	HD2	TYR	46
HA	SER	47 -	HB2	SER	47
HA	SER	47 -	HB3	SER	47
HN	TYR	48 -	HA	TYR	48
HN	TYR	48 -	CG	TYR	48
HA	TYR	48 -	HB2	TYR	48
HA	TYR	48 -	HB3	TYR	48
HA	TYR	48 -	CG	TYR	48
HB2	TYR	48 -	CG	TYR	48
HB3	TYR	48 -	CG	TYR	48
HN	THR	49 -	HA	THR	49
HB	THR	49 -	QG2	THR	49
HN	ASP-	50 -	HA	ASP-	50
HN	ASP-	50 -	HB2	ASP-	50
HN	ASP-	50 -	QB	ASP-	50
HA	ASP-	50 -	HB3	ASP-	50
HA	ASP-	50 -	HN	ALA	51
HN	ALA	51 -	HA	ALA	51
HA	ALA	51 -	QB	ALA	51
HA	ALA	51 -	HN	ASN	52
HN	ASN	52 -	HA	ASN	52
HA	ASN	52 -	HB2	ASN	52
HA	ASN	52 -	HB3	ASN	52
HN	ILE	53 -	HA	ILE	53
HA	ILE	53 -	HB	ILE	53
HA	ILE	53 -	HN	LYS+	54

HG13	ILE	53	-	QD1	ILE	53		HB3	PRO	71	-	HG3	PRO	71
HN	LYS+	54	-	HA	LYS+	54		HG3	PRO	71	-	HD3	PRO	71
HA	LYS+	54	-	HB2	LYS+	54		HN	TML	72	-	HA	TML	72
HA	LYS+	54	-	HN	LYS+	55		HA	TML	72	-	HN	LYS+	73
HN	LYS+	55	-	HA	LYS+	55		HN	LYS+	73	-	HA	LYS+	73
HN	ASN	56	-	HA	ASN	56		HA	LYS+	73	-	HN	TYR	74
HA	ASN	56	-	HB2	ASN	56		HN	TYR	74	-	CG	TYR	74
HA	ASN	56	-	HB3	ASN	56		HA	TYR	74	-	HB2	TYR	74
HN	VAL	57	-	HA	VAL	57		HA	TYR	74	-	HB3	TYR	74
HN	VAL	57	-	QG1	VAL	57		HA	TYR	74	-	CG	TYR	74
HA	VAL	57	-	QG1	VAL	57		HA	TYR	74	-	HN	ILE	75
HA	VAL	57	-	QG2	VAL	57		HB2	TYR	74	-	CG	TYR	74
HB	VAL	57	-	QG1	VAL	57		HB3	TYR	74	-	CG	TYR	74
HB	VAL	57	-	QG2	VAL	57		CG	TYR	74	-	CZ	TYR	74
HN	LEU	58	-	HA	LEU	58		HN	ILE	75	-	HA	ILE	75
HA	LEU	58	-	HB2	LEU	58		HN	ILE	75	-	QG2	ILE	75
HB3	LEU	58	-	QD1	LEU	58		HA	ILE	75	-	HB	ILE	75
HN	TRP	59	-	HA	TRP	59		HA	ILE	75	-	QG2	ILE	75
HN	TRP	59	-	HB3	TRP	59		HA	ILE	75	-	QD1	ILE	75
HA	TRP	59	-	HB2	TRP	59		HB	ILE	75	-	QG2	ILE	75
HB2	TRP	59	-	HD1	TRP	59		HB	ILE	75	-	HG12	ILE	75
HB2	TRP	59	-	HE3	TRP	59		HG12	ILE	75	-	QD1	ILE	75
HB3	TRP	59	-	HD1	TRP	59		HG13	ILE	75	-	QD1	ILE	75
HB3	TRP	59	-	HE3	TRP	59		HA	PRO	76	-	HB2	PRO	76
HD1	TRP	59	-	HE1	TRP	59		HA	PRO	76	-	HB3	PRO	76
HE3	TRP	59	-	HZ3	TRP	59		HA	PRO	76	-	HG3	PRO	76
HE1	TRP	59	-	HZ2	TRP	59		HA	PRO	76	-	HN	GLY	77
HZ3	TRP	59	-	HH2	TRP	59		HB3	PRO	76	-	HG3	PRO	76
HZ2	TRP	59	-	HH2	TRP	59		HB3	PRO	76	-	HD3	PRO	76
HN	GLU-	61	-	HA	GLU-	61		HG3	PRO	76	-	HD3	PRO	76
HA	GLU-	61	-	HB2	GLU-	61		HA1	GLY	77	-	HN	THR	78
HA	GLU-	61	-	HB3	GLU-	61		HA2	GLY	77	-	HN	THR	78
HA	GLU-	61	-	HN	ASN	62		HN	THR	78	-	HA	THR	78
HN	ASN	62	-	HA	ASN	62		HA	THR	78	-	HN	LYS+	79
HA	ASN	62	-	HB2	ASN	62		HB	THR	78	-	QG2	THR	78
HA	ASN	62	-	HB3	ASN	62		HB	THR	78	-	HG1	THR	78
HA	ASN	62	-	HN	ASN	63		QG2	THR	78	-	HG1	THR	78
HB3	ASN	62	-	HD21	ASN	62		HN	LYS+	79	-	HA	LYS+	79
HN	ASN	63	-	HA	ASN	63		HN	LYS+	79	-	HB3	LYS+	79
HA	ASN	63	-	HB3	ASN	63		HA	LYS+	79	-	HG3	LYS+	79
HA	ASN	63	-	HN	MET	64		HA	LYS+	79	-	HN	MET	80
HB2	ASN	63	-	HD21	ASN	63		HB3	LYS+	79	-	HG3	LYS+	79
HB3	ASN	63	-	HD21	ASN	63		HN	ALA	81	-	HA	ALA	81
HN	MET	64	-	HA	MET	64		HA	ALA	81	-	QB	ALA	81
HN	MET	64	-	HB2	MET	64		HN	PHE	82	-	HB2	PHE	82
HA	MET	64	-	HB3	MET	64		HB2	PHE	82	-	QR	PHE	82
HA	MET	64	-	HN	SER	65		HB3	PHE	82	-	QR	PHE	82
HN	SER	65	-	HA	SER	65		HZ	PHE	82	-	QR	PHE	82
HA	SER	65	-	HN	GLU-	66		HN	LEU	85	-	HA	LEU	85
HN	GLU-	66	-	HA	GLU-	66		HN	LEU	85	-	HB3	LEU	85
HA	GLU-	66	-	HN	TYR	67		HA	LEU	85	-	HB3	LEU	85
HN	TYR	67	-	HA	TYR	67		HB2	LEU	85	-	QD1	LEU	85
HA	TYR	67	-	HB2	TYR	67		HB3	LEU	85	-	QD1	LEU	85
HA	TYR	67	-	HB3	TYR	67		HB3	LEU	85	-	QD2	LEU	85
HA	TYR	67	-	CG	TYR	67		HG	LEU	85	-	QD1	LEU	85
HA	TYR	67	-	HN	LEU	68		HN	LYS+	86	-	HA	LYS+	86
HB2	TYR	67	-	CG	TYR	67		HA	LYS+	86	-	HB2	LYS+	86
HB3	TYR	67	-	CG	TYR	67		HA	LYS+	86	-	HN	LYS+	87
HN	LEU	68	-	HA	LEU	68		HN	LYS+	87	-	HA	LYS+	87
HA	LEU	68	-	HB2	LEU	68		HN	GLU-	88	-	HA	GLU-	88
HA	LEU	68	-	HB3	LEU	68		HA	GLU-	88	-	HB2	GLU-	88
HA	LEU	68	-	HN	THR	69		HN	LYS+	89	-	HA	LYS+	89
HB2	LEU	68	-	QD1	LEU	68		HA	ASP-	90	-	HB2	ASP-	90
HB2	LEU	68	-	QD2	LEU	68		HA	ASP-	90	-	HB3	ASP-	90
HB3	LEU	68	-	QD1	LEU	68		HN	ARG+	91	-	HA	ARG+	91
HB3	LEU	68	-	QD2	LEU	68		HA	ARG+	91	-	HB2	ARG+	91
HG	LEU	68	-	QD1	LEU	68		HA	ARG+	91	-	HN	ASN	92
HG	LEU	68	-	QD2	LEU	68		HN	ASN	92	-	HA	ASN	92
HN	THR	69	-	HA	THR	69		HA	ASN	92	-	HN	ASP-	93
HN	THR	69	-	QG2	THR	69		HN	ASP-	93	-	HA	ASP-	93
HA	THR	69	-	HB	THR	69		HA	ASP-	93	-	HB3	ASP-	93
HA	THR	69	-	QG2	THR	69		HA	ASP-	93	-	HN	LEU	94
HA	THR	69	-	HN	ASN	70		HN	LEU	94	-	HA	LEU	94
HB	THR	69	-	QG2	THR	69		HA	LEU	94	-	HN	ILE	95
HN	ASN	70	-	HA	ASN	70		HB2	LEU	94	-	QD2	LEU	94
HN	ASN	70	-	HB2	ASN	70		HB3	LEU	94	-	HG	LEU	94
HA	ASN	70	-	HB2	ASN	70		HB3	LEU	94	-	QD2	LEU	94
HA	ASN	70	-	HB3	ASN	70		HG	LEU	94	-	QD1	LEU	94
HA	PRO	71	-	HB2	PRO	71		HG	LEU	94	-	QD2	LEU	94
HA	PRO	71	-	HG3	PRO	71		HN	ILE	95	-	HA	ILE	95
HA	PRO	71	-	HD2	PRO	71		HA	ILE	95	-	HB	ILE	95
HA	PRO	71	-	HN	TML	72		HA	ILE	95	-	QG2	ILE	95

HA	ILE	95	-	QD1	ILE	95
HB	ILE	95	-	QG2	ILE	95
HB	ILE	95	-	HG13	ILE	95
HB	ILE	95	-	QD1	ILE	95
HG12	ILE	95	-	QD1	ILE	95
HG13	ILE	95	-	QD1	ILE	95
HN	THR	96	-	HA	THR	96
HN	THR	96	-	QG2	THR	96
HB	THR	96	-	QG2	THR	96
HN	TYR	97	-	HA	TYR	97
HA	TYR	97	-	HN	LEU	98
HD1	TYR	97	-	HE1	TYR	97
HN	LEU	98	-	HA	LEU	98
HA	LEU	98	-	HN	LYS+	99
HB2	LEU	98	-	QD1	LEU	98
HB2	LEU	98	-	QD2	LEU	98
HB3	LEU	98	-	QD1	LEU	98
HB3	LEU	98	-	QD2	LEU	98
HG	LEU	98	-	QD1	LEU	98
HG	LEU	98	-	QD2	LEU	98
HN	LYS+	99	-	HA	LYS+	99
HA	LYS+	99	-	HB2	LYS+	99
HA	LYS+	99	-	HB3	LYS+	99
HN	LYS+	100	-	HA	LYS+	100
HA	LYS+	100	-	HN	ALA	101
HN	ALA	101	-	HA	ALA	101
HA	ALA	101	-	QB	ALA	101
HN	GLU-	103	-	HA	GLU-	103

H-bond constraints

10 PHE					
	HN	6	ALA	O	2.40
	N	6	ALA	O	2.70-3.40
11 LYS+					
	HN	8	ALA	O	2.40
	N	8	ALA	O	2.70-3.40
15 LEU					
	HN	10	PHE	O	2.40
	N	10	PHE	O	2.70-3.40
31 ASN					
	HN	26	HIS	ND1	2.40
	N	26	HIS	ND1	2.70-3.40
54 LYS+					
	HN	50	ASP-	O	2.40
	N	50	ASP-	O	2.70-3.40
68 LEU					
	HN	64	MET	O	2.40
	N	64	MET	O	2.70-3.40
70 ASN					
	HN	67	TYR	O	2.40
	N	67	TYR	O	2.70-3.40
74 TYR					
	HN	70	ASN	O	2.40
	N	70	ASN	O	2.70-3.40
78 THR					
	HN	75	ILE	O	2.40
	N	75	ILE	O	2.70-3.40
94 LEU					
	HN	90	ASP-	O	2.40
	N	90	ASP-	O	2.70-3.40
97 TYR					
	HN	93	ASP-	O	2.40
	N	93	ASP-	O	2.70-3.40
98 LEU					
	HN	94	LEU	O	2.40
	N	94	LEU	O	2.70-3.40
99 LYS+					
	HN	95	ILE	O	2.40
	N	95	ILE	O	2.70-3.40
101 ALA					
	HN	97	TYR	O	2.40
	N	97	TYR	O	2.70-3.40

Structural constraints from the experimental pseudocontact shifts in ppm

-3	PHE	HD1	-0.19 2
-3	PHE	HD2	-0.19
-3	PHE	HE1	-0.22 2
-3	PHE	HE2	-0.22
-3	PHE	HA	-0.14
-3	PHE	HN	-0.21
-3	PHE	HZ	-0.18
-2	LYS	HA	-0.09
-2	LYS	HN	-0.13
-1	ALA	HA	-0.14
-1	ALA	HN	-0.10
-1	ALA	HB1	-0.12 3
-1	ALA	HB2	-0.12
-1	ALA	HB3	-0.12
1	GLY	HN	-0.20
2	SER	HA	-0.15
2	SER	HN	-0.19
3	ALA	HA	-0.22
3	ALA	HB1	-0.09 3
3	ALA	HB2	-0.09
3	ALA	HB3	-0.09
4	LYS	HN	-0.18
5	LYS	HA	-0.22
5	LYS	HN	-0.20
6	GLY	HN	-0.19
7	ALA	HA	-0.07
7	ALA	HN	-0.13
7	ALA	HB1	-0.02 3
7	ALA	HB2	-0.02
7	ALA	HB3	-0.02
8	THR	HA	-0.08
8	THR	HB	-0.14
8	THR	HN	-0.10
8	THR	HG21	-0.10 3
8	THR	HG22	-0.10
8	THR	HG23	-0.10
9	LEU	HA	-0.37
9	LEU	HG	-0.37
9	LEU	HN	-0.26
10	PHE	HD1	0.02 2
10	PHE	HD2	0.02
10	PHE	HA	-0.59
10	PHE	HN	-0.28
10	PHE	HZ	2.31
11	LYS	HA	0.28
11	LYS	HN	0.07
12	THR	HA	-0.05
12	THR	HN	-0.16
12	THR	HG21	-0.11 3
12	THR	HG22	-0.11
12	THR	HG23	-0.11
13	ARG	HA	-0.63
13	ARG	HN	-0.45
15	LEU	HA	1.96
15	LEU	HG	0.79
15	LEU	HN	0.77
16	GLN	HA	0.76
16	GLN	HN	1.08
19	THR	HA	1.64
19	THR	HB	1.05
19	THR	HN	2.88
19	THR	HG21	1.10 3
19	THR	HG22	1.10
19	THR	HG23	1.10
20	VAL	HA	0.99
20	VAL	HB	0.83
20	VAL	HN	0.94
21	GLU	HA	0.36
21	GLU	HN	1.18
22	LYS	HA	0.54
22	LYS	HN	0.42
23	GLY	HN	0.36
24	GLY	HN	0.43
25	PRO	HA	0.36
26	HIS	HA	0.64
26	HIS	HD2	-0.04
26	HIS	HE1	0.11
27	LYS	HA	0.19
27	LYS	HN	0.62
28	VAL	HA	-0.91
28	VAL	HB	-0.74
28	VAL	HN	0.46
28	VAL	HG11	-2.15 3
28	VAL	HG12	-2.15
28	VAL	HG13	-2.15

28	VAL	HG21	-0.49	3
28	VAL	HG22	-0.49	
28	VAL	HG23	-0.49	
29	GLY	HN	-0.09	
30	PRO	HA	0.21	
30	PRO	HB2	0.08	
30	PRO	HB3	-0.64	
31	ASN	HA	1.79	
31	ASN	HB2	0.56	
31	ASN	HB3	0.78	
31	ASN	HN	0.88	
32	LEU	HA	0.82	
32	LEU	HN	1.69	
32	LEU	HD11	2.38	3
32	LEU	HD12	2.38	
32	LEU	HD13	2.38	
32	LEU	HD21	1.50	3
32	LEU	HD22	1.50	
32	LEU	HD23	1.50	
33	HIS	HA	0.29	
33	HIS	HN	0.61	
34	GLY	HN	0.02	
35	ILE	HA	-0.07	
35	ILE	HB	-0.04	
35	ILE	HN	-0.07	
35	ILE	HD11	-0.54	3
35	ILE	HD12	-0.54	
35	ILE	HD13	-0.54	
35	ILE	HG21	-0.26	3
35	ILE	HG22	-0.26	
35	ILE	HG23	-0.26	
36	PHE	HD1	-0.26	2
36	PHE	HD2	-0.26	
36	PHE	HE1	-0.39	2
36	PHE	HE2	-0.39	
36	PHE	HA	-0.27	
36	PHE	HN	-0.10	
36	PHE	HZ	-0.66	
37	GLY	HN	-0.03	
38	ARG	HA	-0.21	
38	ARG	HN	-0.19	
39	HIS	HA	-0.39	
39	HIS	HD2	-0.14	
39	HIS	HE1	-0.17	
39	HIS	HN	0.12	
40	SER	HA	-0.48	
40	SER	HN	-0.06	
41	GLY	HN	0.67	
42	GLN	HA	-0.19	
42	GLN	HN	-0.45	
43	ALA	HA	-0.09	
43	ALA	HN	-0.61	
43	ALA	HB1	-0.14	3
43	ALA	HB2	-0.14	
43	ALA	HB3	-0.14	
44	GLU	HA	-0.14	
44	GLU	HN	-0.03	
46	TYR	HA	-0.44	
46	TYR	HB2	-1.58	
46	TYR	HB3	0.59	
46	TYR	HD1	0.95	2
46	TYR	HD2	-1.61	
46	TYR	HN	-0.28	
47	SER	HA	-0.48	
48	TYR	HA	-1.10	
48	TYR	HN	-0.47	
49	THR	HA	-0.34	
49	THR	HB	-0.10	
49	THR	HN	-0.68	
49	THR	HG21	-0.34	3
49	THR	HG22	-0.34	
49	THR	HG23	-0.34	
50	ASP	HA	-0.16	
50	ASP	HN	-0.11	
51	ALA	HA	0.15	
51	ALA	HN	0.24	
51	ALA	HB1	0.27	3
51	ALA	HB2	0.27	
51	ALA	HB3	0.27	
52	ASN	HA	0.46	
52	ASN	HN	0.07	
53	ILE	HA	0.23	
53	ILE	HB	-0.02	
53	ILE	HN	-0.07	
53	ILE	HD11	-0.23	3
53	ILE	HD12	-0.23	
53	ILE	HD13	-0.23	
53	ILE	HG21	-0.10	3
53	ILE	HG22	-0.10	
53	ILE	HG23	-0.10	
54	LYS	HA	0.21	
54	LYS	HN	-0.07	
55	LYS	HA	0.19	
55	LYS	HN	-0.10	
56	ASN	HA	-0.02	
56	ASN	HN	0.28	
57	VAL	HA	0.39	
57	VAL	HB	0.30	
57	VAL	HN	-0.10	
58	LEU	HA	-0.00	
58	LEU	HB2	0.02	
58	LEU	HB3	-0.15	
58	LEU	HG	-0.10	
58	LEU	HN	-0.07	
59	TRP	HA	-0.13	
59	TRP	HD1	-0.16	
59	TRP	HE1	-0.13	
59	TRP	HE3	-0.12	
59	TRP	HH2	0.75	
59	TRP	HN	-0.11	
59	TRP	HZ2	0.37	
59	TRP	HZ3	-0.00	
60	ASP	HA	-0.16	
60	ASP	HN	0.34	
61	GLU	HA	-0.34	
61	GLU	HN	-0.28	
62	ASN	HA	-0.16	
62	ASN	HN	-0.10	
63	ASN	HA	0.01	
63	ASN	HN	-0.15	
64	MET	HN	-0.29	
65	SER	HA	-0.43	
65	SER	HN	-0.39	
66	GLU	HA	0.04	
66	GLU	HN	-0.16	
67	TYR	HA	0.60	
67	TYR	HD1	0.31	2
67	TYR	HD2	0.31	
67	TYR	HE1	0.22	2
67	TYR	HE2	0.22	
67	TYR	HN	0.00	
68	LEU	HA	-0.13	
68	LEU	HG	-1.34	
68	LEU	HN	-0.20	
69	THR	HA	-0.05	
69	THR	HB	0.14	
69	THR	HN	0.05	
69	THR	HG21	0.06	3
69	THR	HG22	0.06	
69	THR	HG23	0.06	
70	ASN	HA	0.71	
70	ASN	HN	0.59	
71	PRO	HB2	4.15	
72	TML	HA	1.38	
72	TML	HN	1.70	
73	LYS	HA	0.52	
73	LYS	HN	0.86	
74	TYR	HD1	0.56	2
74	TYR	HD2	0.56	
74	TYR	HE1	0.26	2
74	TYR	HE2	0.26	
74	TYR	HA	0.49	
74	TYR	HN	0.85	
75	ILE	HA	0.68	
75	ILE	HB	1.48	
75	ILE	HN	1.21	
76	PRO	HA	0.63	
77	GLY	HN	0.57	
78	THR	HA	0.56	
78	THR	HB	1.50	
78	THR	HN	0.80	
78	THR	HG21	2.52	3
78	THR	HG22	2.52	
78	THR	HG23	2.52	

79	LYS	HA	0.55	
79	LYS	HN	-0.71	
81	ALA	HA	1.12	
81	ALA	HN	-0.09	
81	ALA	HB1	-0.11	3
81	ALA	HB2	-0.11	
81	ALA	HB3	-0.11	
82	PHE	HA	0.21	
82	PHE	HN	2.46	
82	PHE	HZ	-1.30	
84	GLY	HN	-1.68	
85	LEU	HA	-0.39	
85	LEU	HG	-0.94	
85	LEU	HN	-0.36	
86	LYS	HA	-0.10	
86	LYS	HN	-0.26	
87	LYS	HA	-0.13	
87	LYS	HN	-0.17	
88	GLU	HA	-0.23	
88	GLU	HN	-0.22	
89	LYS	HA	-0.19	
89	LYS	HN	-0.20	
90	ASP	HA	-0.35	
90	ASP	HN	-0.28	
91	ARG	HA	-0.68	
91	ARG	HN	-0.37	
92	ASN	HA	-0.20	
92	ASN	HN	-0.33	
93	ASP	HA	-0.28	
93	ASP	HN	-0.31	
94	LEU	HA	-0.54	
94	LEU	HB2	-0.74	
94	LEU	HB3	-0.94	
94	LEU	HN	-0.51	
95	ILE	HA	-0.68	
95	ILE	HB	-0.46	
95	ILE	HN	-0.60	
95	ILE	HD11	-0.56	3
95	ILE	HD12	-0.56	
95	ILE	HD13	-0.56	
95	ILE	HG21	-0.41	3
95	ILE	HG22	-0.41	
95	ILE	HG23	-0.41	
96	THR	HA	-0.22	
96	THR	HB	-0.27	
96	THR	HN	-0.34	
96	THR	HG21	-0.16	3
96	THR	HG22	-0.16	
96	THR	HG23	-0.16	
97	TYR	HA	-0.16	
97	TYR	HN	-0.31	
98	LEU	HA	-0.16	
98	LEU	HN	-0.44	
99	LYS	HA	-0.15	
99	LYS	HN	-0.26	
100	LYS	HA	-0.05	
100	LYS	HN	-0.13	
101	ALA	HA	0.09	
101	ALA	HN	-0.06	
101	ALA	HB1	0.12	3
101	ALA	HB2	0.12	
101	ALA	HB3	0.12	
102	SER	HN	-0.05	
103	GLU	HA	0.04	
103	GLU	HN	0.05	